

December 24, 2003



**Via US Mail and e-mail**

Mr. Mike Leavitt, Administrator  
U.S. Environmental Protection Agency  
P.O. Box 1473  
Merrifield, VA 2211

**201-15031**

**Re: Specialty Acrylates & Methacrylates (SAM) Panel  
HPV Chemical Challenge Program Submission  
2-Propenoic Acid, Isodecyl Ester (CAS number 1330-61-6)  
Test Plan and Data Review**

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Dear Mr. Leavitt:

The SAM Panel of the American Chemistry Council is pleased to submit the attached documents to the High Production Volume (HPV) Chemical Challenge Program (Program) to fulfill our commitment for 2-Propenoic Acid, Isodecyl Ester (commonly known as Isodecyl acrylate or IDA; CAS number 1330-61-6), which the SAM Panel is voluntarily sponsoring in the Program. Members of the SAM Panel are: Akzo Nobel Resins, Atofina, BASF Corporation, Ciba Specialty Chemicals, Cognis Corporation, Mitsubishi Gas Chemicals USA, Rhodia, Röhm GmbH, RohMax-USA, San Esters, Sartomer Corporation and UCB.

The submission consists of the *Test Plan and Data Review* and robust summaries in a IUCLID-format file for IDA.

This submission also is being sent electronically to the following e-mail addresses:

Oppt.ncic@epa.gov  
Chem.rtk@epa.gov

If you require additional information, please contact the SAM Panel's technical contact, Dr. Anne P. LeHuray at (703) 741-5630 or [anne\\_lehuray@americanchemistry.com](mailto:anne_lehuray@americanchemistry.com).

Sincerely yours,

Attachments



Responsible Care®

**201-15031A**

**2-Propenoic Acid, Isodecyl Ester**

**(Isodecyl Acrylate; CAS RN 1330-61-6)**

**High Production Volume (HPV) Chemical  
Challenge Test Plan and Data Review**

Prepared for:

**ACC Specialty Acrylates and Methacrylates Panel**

Prepared by:

**Toxicology/Regulatory Services, Inc.**

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**2-Propenoic Acid, Isodecyl Ester**  
**High Production Volume Chemical Challenge**  
**Test Plan and Data Review**

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### Test Plan

2-Propenoic Acid, Isodecyl Ester (Isodecyl Acrylate; CAS RN: 1330-61-6)		Information	OECD Study	GLP	Other Study	Estimation Method	Acceptable	Testing Required
STUDY		Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
IUCLID #	PHYSICAL AND CHEMICAL DATA							
2.1	Melting Point	Y	N	N	Y	N	Y	N
2.2	Boiling Point	Y	N	N	Y	N	Y	N
2.4	Vapor Pressure	Y	N	N	Y	N	Y	N
2.5	Partition Coefficient	Y	N	N	N	Y	Y	N
2.6	Water Solubility	Y	N	N	Y	Y	Y	N
IUCLID #	ENVIRONMENTAL FATE AND PATHWAY							
3.1.1	Photodegradation	Y	N	N	N	Y	Y	N
3.1.2	Stability in Water	Y	N	N	Y	N	Y	N
3.3	Transport and Distribution	Y	N	N	N	Y	Y	N
3.5	Biodegradation	Y	Y	N	N	N	Y	N
IUCLID #	ECOTOXICITY							
4.1	Acute Toxicity to Fish	Y	Y	N	N	N	Y	N
4.2	Toxicity to Daphnia	Y	Y	N	N	N	Y	N
4.3	Acute Toxicity to Algae	Y	Y	N	N	N	Y	N
IUCLID #	TOXICITY							
5.1	Acute Toxicity	Y	Y	Y	N	N	Y	N
5.4	Repeated Dose Toxicity	Y	Y	Y	N	N	Y	N
5.5	Genotoxicity <i>In Vitro</i> (Bacterial Test)	Y	Y	N	N	N	Y	N
5.5	Genotoxicity <i>In Vitro</i> (Mammalian Cells)	Y	Y	Y	N	N	Y	N
5.8	Reproductive Toxicity	Y	Y	Y	N	N	Y	N
5.9	Development Toxicity / Teratogenicity	Y	Y	Y	N	N	Y	N

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**2-Propenoic Acid, Isodecyl Ester  
(Isodecyl Acrylate; CAS RN 1330-61-6)  
High Production Volume Chemical Challenge  
Test Plan and Data Review**

**1.0 Introduction**

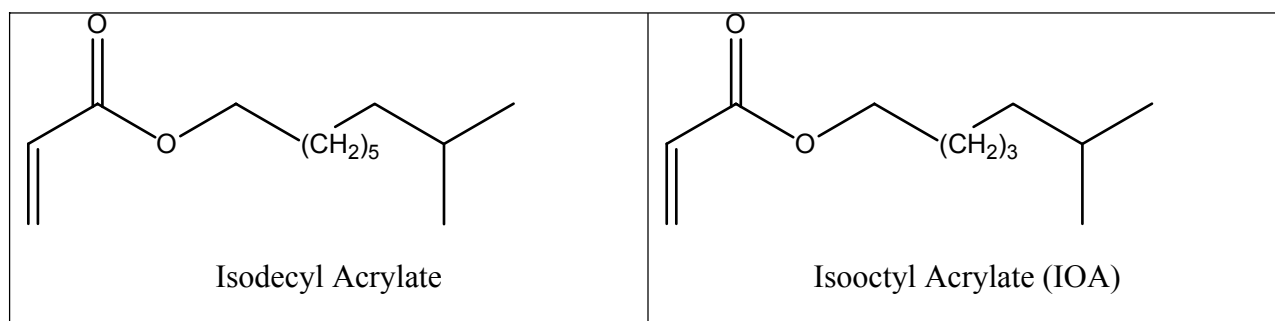
This document provides a Test Plan and reviews the data availability for the High Production Volume (HPV) Chemical Challenge Program (Program) endpoints for 2-Propenoic Acid, Isodecyl Ester, hereafter called Isodecyl Acrylate [CAS RN 1330-61-6], for the American Chemistry Council's Specialty Acrylates and Methacrylates Panel. The availability of adequate data applicable to Isodecyl Acrylate for Program endpoints is summarized in the Test Plan table.

**2.0 General Use and Exposure**

Isodecyl Acrylate is manufactured as an intermediate used for the synthesis of acrylic polymers. Applications include wood and vinyl coatings for floorings, pressure sensitive adhesives, paper coatings, release coatings, optical coatings and screen inks. Isodecyl Acrylate is used in ultraviolet and electron beam (UV/EB) curing processes for production of polymers. UV/EB processes are low-energy technologies that eliminate or greatly reduce the need for volatile organic solvents. In addition, curing rates are very rapid and the reactions virtually complete such that residual monomer is negligible in the final product. Occupational exposure may occur either as the liquid or vapor. Ventilation systems are used to limit vapor exposure. Air monitoring studies reported in the SIAR for the closely related isooctyl acrylate (IOA), for processing and manufacturing areas have typically indicated airborne concentrations to be below the limit of detection. Since Isodecyl Acrylate is slightly less volatile than IOA, inhalation exposure to workers is not anticipated. Federal regulations require impermeable gloves to be worn by all employees who may come into contact with unreacted monomer. Based on the high cross-linking and very low residual monomer in finished products, consumer exposure to Isodecyl Acrylate is not anticipated.

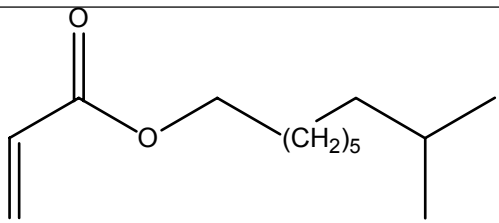
**3.0 Justification for Use of Isooctyl Acrylate (IOA) Data to Support Isodecyl Acrylate**

Isodecyl Acrylate and Isooctyl Acrylate (CAS number 29590-42-9), hereafter referred to as IOA, are very similar congeners of a large family of closely related acrylic acid esters. They are comprised of long-chain hydrocarbon esters with terminal branching. The two chemicals are hydrophobic and similar in general physical/chemical and toxicological properties, and belong to the larger category of physically and toxicologically similar chemicals known as the Specialty Acrylates and Methacrylate Category. The structures of these two acrylate esters are shown below.



The Organization for Economic Cooperation and Development (OECD) has completed a Screening Information Data Set (SIDS) assessment on IOA (SIDS, Volume 1, Part 2) and key studies for HPV Program endpoints are summarized in the SIDS Initial Assessment Report (SIAR) for IOA that accompanies this Test Plan. The OECD evaluation concluded: “Based on its low occupational exposure potential, its low toxicity in in vitro and mammalian studies, its limited release to the environment and its predicted rapid environmental biodegradation, IOA is considered a low priority for additional human health or environmental effects testing at this time.” As shown below and throughout this document, the physical/chemical properties, use patterns, potential environmental releases, and worker safety procedures are essentially the same for Isodecyl Acrylate and IOA. Therefore, this HPV Program test plan uses IOA data extensively in support of the HPV/SIDS endpoints for Isodecyl Acrylate.

#### 4.0 General Substance Information (Identity)

Chemical Name	2-Propenoic Acid, Isodecyl Ester
Synonyms	Acrylic acid, Isodecyl ester Isodecyl acrylate Isodecyl alcohol, acrylate Isodecyl propenoate
CAS Number	1330-61-6
Structure	
Molecular Weight	212.32
Substance Type	Organic
Physical State	Clear Liquid

## 5.0 **Physical/Chemical Properties**

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The robust summaries are included in the attached IUCLID-format document.

### 5.1 Melting Point

The melting point for Isodecyl Acrylate from Handbook data (Lide, 1996) and from the Experimental Database for EPIWIN (U.S. EPA, 2000a) is -100° C. No data were included in the accepted SIAR for IOA. The EPIWIN estimated melting point for Isodecyl Acrylate and IOA is 11.5 and -10.4 °C, respectively. These data are considered adequate to meet the HPV Program requirements.

### 5.2 Boiling Point

The boiling point for Isodecyl Acrylate from Handbook data (Lide, 1996) and from the Experimental Database for EPIWIN (U.S. EPA, 2000a) is 158 °C. The boiling point accepted in the SIAR for IOA is 196.8 °C. The EPIWIN estimated boiling point for Isodecyl Acrylate and IOA is 253.4 and 216.9 °C, respectively. The determination of the boiling point of IOA, Isodecyl Acrylate and other mono- and multi-functional acrylates is of minimal value. The double bond in these chemicals is so reactive that boiling them at atmospheric pressure results in polymerization and decomposition. As a result, these substances are not boiled at atmospheric pressure in normal manufacture or use. Moreover, distillation under vacuum at a lower temperature would generate a pure substance, since the inhibitor would be left behind. Without an inhibitor present, the pure substances quickly polymerize, even at room temperature. Therefore, the available data are considered adequate to meet the HPV Program requirements.

### 5.3 Vapor Pressure

The literature referenced (Howard and Meylan, 1997) and model (U.S. EPA, 2000a) estimate vapor pressure value for Isodecyl Acrylate is 0.03 hPa. The vapor pressure accepted in the SIAR for IOA is 1.33 hPa at 25 °C and the model predicts a vapor pressure of 0.2 hPa. The value of 0.03 hPa is consistent with the large size and known properties of Isodecyl Acrylate. These data are considered adequate to meet the HPV Program requirements.

### 5.4 Partition Coefficient

The literature referenced (Howard and Meylan, 1997) and model (U.S. EPA, 2000b) estimate for the log  $K_{ow}$  value of Isodecyl Acrylate is 5.07 hPa. The log  $K_{ow}$  accepted in the SIAR for IOA is 3.93, and the model predicts a log  $K_{ow}$  value of 4.09. The value of 5.07 is consistent with the hydrophobicity and known properties of Isodecyl Acrylate. These data are considered adequate to meet the HPV Program requirements.

### 5.5 Water Solubility

The reported value for water solubility of IOA that was accepted in the SIAR is 12.44 mg/L at 23.1 °C. The model estimated value (U.S. EPA, 2000c) is very similar, 16.8 mg/L. For

Isodecyl Acrylate, the more hydrophobic ester group, isodecane, will provide for a slightly lower water solubility. The literature referenced (Howard and Meylan, 1997) and model (U.S. EPA, 2000c) estimate value for water solubility of Isodecyl Acrylate of 1.75 mg/L is consistent with the expectation of slightly lower solubility than IOA as well as with the known properties of Isodecyl Acrylate. The robustness of the model value for IOA compared to the measured value provides further support for the accuracy of the model estimate of 1.75 mg/L value for Isodecyl Acrylate. These data are considered adequate to meet the HPV Program requirements.

## 6.0 **Environmental Fate**

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The robust summaries are included in the attached IUCLID-format document.

### 6.1 Photodegradation

The model prediction for atmospheric photodegradation of Isodecyl Acrylate provides a second order rate of reaction with hydroxyl radicals of  $22.2 \times 10^{-12} \text{ cm}^3/\text{molecule-sec}$  and a  $t_{1/2}$  of 5.8 hours (U.S. EPA, 2000d). Similar values are estimated for IOA,  $19.4 \times 10^{-12} \text{ cm}^3/\text{molecule-sec}$  and 6.6 hours. These data are considered adequate to meet the HPV Program requirements.

### 6.2 Stability in Water

Esters of acrylate and methacrylate are all hydrolytically stable at acidic and neutral pH. At approximately pH 11, these molecules rapidly (generally with  $t_{1/2}$  of minutes) hydrolyze to acrylic acid and the appropriate alcohol. A broad database exists supporting this pH-dependent hydrolysis for these types of molecules, much of which has been submitted in the HPV Chemicals Challenge Program, the OECD SIDS program and others. The pH range relevant to determination of environmental fate is generally between pH 5 and 7. Therefore, hydrolysis is not a significant route of degradation in the environment and additional testing will not further the understanding of the environmental fate of Isodecyl Acrylate. The model is not accurate for determination of hydrolysis but does 'recognize' the hydrolytic stability of the molecule indicating half lives of > 1 year at pH 7 and 8. Based on the extensive background data for acrylic and methacrylic esters, these data are considered adequate to meet the HPV Program requirements.

### 6.3 Transport and Distribution

Potential environmental exposure to Isodecyl Acrylate is limited based on the use patterns in UV/EB coating applications and the minimal residual monomer levels in final product polymers. Therefore, only accidental releases were considered for the fugacity modeling (U.S. EPA, 2000e). Two scenarios, 100% release to air and 100% release to water were examined. For the air release, the model predicted a distribution of 96% into atmosphere, 1.6% into water, 1% into soil, and 1% into sediment. For the water release, the model predicted a distribution of 1.5% into atmosphere, 60% into water, <0.1% into soil, and 39% into sediment. For completeness, similar estimates were made for IOA (these data were not taken from the accepted SIAR). For the air release of IOA, the model predicted a distribution

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of 96% into atmosphere, 3% into water, 1% into soil, and <1% into sediment. For the water release, the model predicted a distribution of 2.4% into atmosphere, 91% into water, <0.1% into soil, and 7% into sediment. These data are considered adequate to meet the HPV Program requirements.

#### 6.4 Biodegradability

As defined in the accepted SIAR, IOA has been shown to be rapidly degraded in an OECD 301D test (72% degradation in 5 days and 100% degradation in 28 days) and is Readily Biodegradable (3M unpublished data). The similar structure of Isodecyl Acrylate indicates that it will also undergo rapid biodegradation in the environment. In addition, the closely related, Isodecyl Methacrylate (submitted in the Hydrophobic Methacrylate Category for ICCA), degraded 88% in 28 days although the 10-day window was not met (Elf Atochem, 2001). These data are considered adequate to meet the HPV Program requirements.

### 7.0 Ecotoxicity

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The robust summaries are included in the attached IUCLID-format document.

#### 7.1 Toxicity to Fish

The 96-hour LC<sub>50</sub> value for the fathead minnow accepted for IOA in the SIAR is 0.67 mg/L (3M unpublished data). Although the water solubility is slightly lower for Isodecyl Acrylate, this value is adequate for the screening nature of the HPV Program and indicates that Isodecyl Acrylate is toxic to fish. The ECOSAR submodel of EPIWIN (U.S. EPA, 2000f) predicts an LC<sub>50</sub> value of 0.9 mg/L for Isodecyl Acrylate consistent with the anticipated toxicity based on the value for IOA. These data are considered adequate to meet the HPV Program requirements.

#### 7.2 Toxicity to Aquatic Invertebrates

The 48-hour EC<sub>50</sub> value for *Daphnia magna* accepted for IOA in the SIAR is 0.4 mg/L (3M unpublished data). Although the water solubility is slightly lower for Isodecyl Acrylate, this value is adequate for the screening nature of the HPV Program and indicates that Isodecyl Acrylate is toxic to aquatic invertebrates. The ECOSAR submodel of EPIWIN (U.S. EPA, 2000f) predicts an EC<sub>50</sub> value of 0.55 mg/L for Isodecyl Acrylate consistent with the anticipated toxicity based on the value for IOA. These data are considered adequate to meet the HPV Program requirements.

#### 7.3 Toxicity to Aquatic Plants

The 96-hour EC<sub>50</sub> value for algae accepted for IOA in the SIAR is 2.13 mg/L (3M unpublished data). Although the water solubility is slightly lower for Isodecyl Acrylate, this value is adequate for the screening nature of the HPV Program and indicates that Isodecyl Acrylate is toxic to aquatic invertebrates. The ECOSAR submodel of EPIWIN (U.S. EPA, 2000f) predicts an EC<sub>50</sub> value of 0.066 mg/L for Isodecyl Acrylate predicting greater toxicity than expected from the value for IOA. These data are considered adequate to meet the HPV Program requirements.

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#### 7.4 Chronic Toxicity to Aquatic Invertebrates

IOA was tested in two reproduction studies with *Daphnia magna* that were accepted as part of the SIAR review. The EC<sub>50</sub> values for reproduction in these studies were 1.99 and 1.61 mg/L (3M, unpublished data) confirming that IOA and Isodecyl Acrylate, by analogy, are toxic to aquatic invertebrates. These data are considered adequate to meet the HPV Program requirements.

### 8.0 Human Health-Related Data

A data summary for Isodecyl Acrylate and IOA is included in Table 1. The robust summaries are included in the attached IUCLID-format document. The studies summarized below and in the robust summaries are for IOA.

#### 8.1 Acute Toxicity

The acute oral LD<sub>50</sub> in rats for IOA accepted for the SIAR is > 5000 mg/kg body weight (Glaza, 1989; Gordon *et al.*, 1991). This value is consistent with the limited toxicity of hydrophobic acrylate and methacrylate esters and is considered appropriate for Isodecyl Acrylate. These data are considered adequate to meet the HPV Program requirements.

#### 8.2 Repeated Dose Toxicity

IOA was tested using the OECD 422 Combined Repeat Dose and Reproductive/Developmental Screening Test (Henwood, 1993) that was accepted for the SIAR. In this test, male and female Fischer 344 rats were treated with 1.0%, 7.5%, 15%, or 25% (lowered to 20% after 1 week) IOA in acetone at a dose volume of 100 µL/day for two weeks prior to breeding and during breeding, gestation, and through postnatal day 4. Dermal irritation, consisting of moderate erythema, slight desquamation, and slight fissuring (females only) was observed in the high dose group. Slight increases in serum aspartate aminotransferase and alanine aminotransferase concentrations were noted in males from the high dose group. No other treatment-related effects were observed. Based on the very limited systemic effects in this study and recognizing that the primary route of potential exposure to Isodecyl Acrylate is via skin contact, these data are adequate to support the conclusion that no significant toxicity is anticipated from dermal exposure under current use patterns to Isodecyl Acrylate. Therefore, the available data are considered adequate to meet the HPV Program requirements.

#### 8.3 Genetic Toxicity

##### 8.3.1 *In vitro*

IOA was tested in a bacterial gene mutation assay according to OECD Guideline 471 with Salmonella strains TA1535, TA1537, TA1538, TA98 and TA100. IOA was negative with and without metabolic activation at concentrations ranging from 0.005 to 0.5 µL/plate (Mortelmans and Pomeroy, 1980; Gordon *et al.*, 1991).

IOA was tested in a mouse lymphoma assay according to OECD Guideline 476. There was no evidence of mutagenicity in this mammalian cell assay at concentrations ranging from 0.0015 to 0.11 µL/plate (Kirby, 1980; Gordon *et al.*, 1991).

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Isodecyl Acrylate and IOA are members of a large family of acrylic acid esters. A large battery of mutagenicity screening tests exists for these chemicals and the results of these studies have been submitted in other HPV and ICCA Test Plans. The conclusion that these esters are not mutagenic is consistent for the family as a whole. As concluded in the SIAR for IOA, the exposure and low toxicity of these chemicals indicates that further testing will not provide additional knowledge of the potential hazards. Therefore, consistent with the IOA SIAR, the available data are considered adequate to meet the HPV Program requirements.

#### 8.4 Reproductive and Developmental Toxicity

IOA was tested using the OECD 422 Combined Repeat Dose and Reproductive/Developmental Screening Test that was accepted for the SIAR. In this test, male and female Fischer 344 rats were treated with 1.0%, 7.5%, 15%, or 25% (lowered to 20% after 1 week) IOA in acetone at a dose volume of 100  $\mu$ L/day for two weeks prior to breeding and during breeding, gestation, and through postnatal day 4 (see Repeated Dose Toxicity above). There were no treatment-related effects on male fertility, female fertility, mean days to mating, length of gestation, gestation length, pup viability mean number of pups/litter, or pup weights. There were no treatment-related findings at necropsy of the pups. Reproductive organ weight and histopathology findings for the adults were similar to controls. The reproductive and developmental NOAEL was 20%. Based on the lack of effects in this study and recognizing that the primary route of potential exposure to Isodecyl Acrylate is via skin contact, these data are adequate to support the conclusion that no reproductive or developmental toxicity is anticipated from exposure under current use patterns to Isodecyl Acrylate. Therefore, the available data are considered adequate to meet the HPV Program requirements.

### 9.0 Conclusion

Isodecyl Acrylate and IOA are very similar congeners of a large family of acrylic acid esters. The data for IOA have been used extensively in evaluation of the HPV/SIDS endpoints for Isodecyl Acrylate. Adequate information is available for melting point, boiling point, vapor pressure and partition coefficient for both chemicals. Photodegradation and environmental distributions are adequately supported by the appropriate model data for Isodecyl Acrylate and the model data for IOA support the similarity of the chemicals. Hydrolysis of acrylic acid esters does not occur at physiological or environmental pH. The aquatic tests with fish, invertebrates and plants, for IOA indicates that IOA, Isodecyl Acrylate and other hydrophobic acrylic esters are toxic to aquatic organisms. Since IOA and, therefore, Isodecyl Acrylate, rapidly degrades in the environment and environmental exposure is very limited, the degradation and toxicity studies for IOA are adequate to support Isodecyl Acrylate environmental fate and effects. The LD<sub>50</sub> of IOA is >5000 mg/kg and subchronic toxicity evaluations indicate that only skin irritation would be anticipated from exposure to these hydrophobic acrylate esters. IOA is not mutagenic in screening assays consistent with the family of acrylic acid esters. Isodecyl Acrylate, therefore, is also considered not to pose a mutagenic hazard. As with repeated dose studies, evaluation of the reproductive and developmental toxicity of IOA is adequate for Isodecyl Acrylate and indicates that Isodecyl Acrylate does not affect reproduction or the developing offspring. Overall, the available data for IOA, consistent with the conclusions of the SIAM, are considered adequate to meet the HPV Chemical Challenge Program requirements and serve to similarly support Isodecyl Acrylate.

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## 10.0 References

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- Galloway, S. 2000. Cytotoxicity and Chromosomal Aberrations in vitro: Experience in Industry and the Case for an Upper Limit on Toxicity in the Aberration Assay. *Environmental and Molecular Mutagenesis* 35:191-201.
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- U. S. EPA (U.S. Environmental Protection Agency). 2000b. EPI Suite™, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

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- U. S. EPA (U.S. Environmental Protection Agency). 2000c. EPI Suite™, Version 3.11; WSKOW Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- U.S. EPA (U.S. Environmental Protection Agency). 2000d. EPI Suite™, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- U.S. EPA (U.S. Environmental Protection Agency). 2000e. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- U.S. EPA (U.S. Environmental Protection Agency). 2000f. EPI Suite™, Version 3.11; ECOSAR Version 0.99g; PC-Computer software developed by ECOSAR Program, Risk Assessment Division (7403), Washington, D.C.

<b>Table 1: Data Summary</b> <b>2-Propenoic Acid, Isodecyl Ester</b>				
CAS NO: 1330-61-6		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL PROPERTIES				
2.1	Melting Point		Handbook Data – for Isodecyl Acrylate	-100 °C
2.2	Boiling Point		Handbook Data – for Isodecyl Acrylate	158 °C
2.4	Vapor Pressure		Handbook Data – for Isodecyl Acrylate	0.03 hPa (at 20 °C )
2.5	Partition Coefficient (log K <sub>ow</sub> )		KOWWIN v. 1.67 – for Isodecyl Acrylate	5.07
2.6	Water Solubility		WSKOW v. 1.41 – for Isodecyl Acrylate	1.75 mg/L
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		AOPWIN v. 1.91 – for Isodecyl Acrylate	half-life: 5.8 hours (OH Rate Constant)
3.1.2	Stability in Water			Acrylate esters are stable at pH 3 and 7 and hydrolyze rapidly to acrylate and the associated alkyl chain at pH 11.
3.3	Transport and Distribution		Mackay Level III – for Isodecyl Acrylate 100% release to air	96% into atmosphere, 1.6% into water, 1% into soil, 1% into sediment
			Mackay Level III – for Isodecyl Acrylate 100% release to water	1.5% into atmosphere, 60% into water, <0.1% into soil, 39% into sediment
3.5	Biodegradation		OECD 301D – for IOA	100% after 28 days; Readily Biodegradable
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish*	<i>Pimephales promelas</i>	OECD 203 – for IOA	LC <sub>50</sub> (96 hours) = 0.67 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates	<i>Daphnia magna</i>	OECD 202 – for IOA	EC <sub>50</sub> (48 hours) = 0.4 mg/L
4.3	Toxicity to Aquatic Plants e.g. Algae	Green algae	OECD 201 – for IOA	EC <sub>50</sub> (72 hours) = 2.13 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates	<i>Daphnia magna</i>	OECD 202 (2 studies) – for IOA	EC <sub>50</sub> (Reproduction) = 1.99 mg/L EC <sub>50</sub> (Reproduction) = 1.61 mg/L

<b>Table 1: Data Summary</b> <b>2-Propenoic Acid, Isodecyl Ester</b>				
CAS NO: 1330-61-6		SPECIES	PROTOCOL	RESULTS
TOXICOLOGY				
5.1	Acute Oral Toxicity	Rat	OECD 401 – for IOA	LD <sub>50</sub> : >5000 mg/kg bw
5.7	Repeated Dose Toxicity	Rat - Dermal	OECD 422 – for IOA	NOAEL = 15% (100 µl/day)
5.8	Genetic Toxicity <i>In Vitro</i>  Bacterial Test (Gene mutation)	<i>Salmonella typhimurium</i>	OECD 471 – for IOA	Negative
		Mouse lymphoma	OECD 476 – for IOA	Negative
5.11	Toxicity to Reproduction / Impairment of Fertility	Rat - Dermal	OECD 422 – for IOA	NOAEL > 20% (100 µl/day)
5.12	Developmental Toxicity / Teratogenicity	Rat - Dermal	OECD 422 – for IOA	NOAEL > 20% (100 µl/day)

201-15031B1

# I U C L I D

## Data Set

RECEIVED  
OPTIC  
04 JAN 12 PM 3:08

Existing Chemical : ID: 1330-61-6  
CAS No. : 1330-61-6  
EINECS Name : Isodecyl acrylate  
EC No. : 215-542-5  
TSCA Name : 2-Propenoic acid, isodecyl ester  
Molecular Formula : C<sub>13</sub>H<sub>24</sub>O<sub>2</sub>

Producer related part  
Company : ACC Specialty Acrylates and Methacrylates Panel  
Creation date : 29.11.2001

Substance related part  
Company : ACC Specialty Acrylates and Methacrylates Panel  
Creation date : 29.11.2001

Status :  
Memo : Isodecyl

Printing date : 17.12.2003  
Revision date :  
Date of last update : 17.12.2003

Number of pages : 36

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10  
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4  
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),  
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

# 1. General Information

**Id** 1330-61-6  
**Date** 17.12.2003

## 1.0.1 APPLICANT AND COMPANY INFORMATION

## 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

## 1.0.3 IDENTITY OF RECIPIENTS

## 1.0.4 DETAILS ON CATEGORY/TEMPLATE

### 1.1.0 SUBSTANCE IDENTIFICATION

**IUPAC Name** :  
**Smiles Code** : O=C(C=C)OCCCCCCCC(C)C  
**Molecular formula** : C13 H24 O2  
**Molecular weight** : 212.32  
**Petrol class** :

17.12.2003

### 1.1.1 GENERAL SUBSTANCE INFORMATION

**Purity type** : typical for marketed substance  
**Substance type** : organic  
**Physical status** : liquid  
**Purity** : ca. 100 % v/v  
**Colour** : clear  
**Odour** : mild acrylic

17.12.2003

### 1.1.2 SPECTRA

## 1.2 SYNONYMS AND TRADENAMES

Acrylic acid, isodecyl ester  
Isodecyl acrylate  
Isodecyl alcohol, acrylate  
Isodecyl propenoate

16.12.2003

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## 1. General Information

Id 1330-61-6  
Date 17.12.2003

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### 1.3 IMPURITIES

### 1.4 ADDITIVES

### 1.5 TOTAL QUANTITY

### 1.6.1 LABELLING

### 1.6.2 CLASSIFICATION

### 1.6.3 PACKAGING

### 1.7 USE PATTERN

### 1.7.1 DETAILED USE PATTERN

### 1.7.2 METHODS OF MANUFACTURE

### 1.8 REGULATORY MEASURES

### 1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

### 1.8.2 ACCEPTABLE RESIDUES LEVELS

### 1.8.3 WATER POLLUTION

### 1.8.4 MAJOR ACCIDENT HAZARDS

## 1. General Information

**Id** 1330-61-6  
**Date** 17.12.2003

**1.8.5 AIR POLLUTION**

**1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES**

**1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS**

**1.9.2 COMPONENTS**

**1.10 SOURCE OF EXPOSURE**

**1.11 ADDITIONAL REMARKS**

**1.12 LAST LITERATURE SEARCH**

**1.13 REVIEWS**

## 2. Physico-Chemical Data

Id 1330-61-6

Date 17.12.2003

### 2.1 MELTING POINT

<b>Value</b>	:	= -100 °C	
<b>Sublimation</b>	:		
<b>Method</b>	:		
<b>Year</b>	:		
<b>GLP</b>	:	no data	
<b>Test substance</b>	:	as prescribed by 1.1 - 1.4	
<b>Source</b>	:	Handbook data Rohm and Haas Company Spring House	
<b>Reliability</b>	:	(2) valid with restrictions	
<b>Flag</b>	:	Critical study for SIDS endpoint	
15.12.2003			(4) (7)
<b>Value</b>	:	= -100 °C	
<b>Sublimation</b>	:		
<b>Method</b>	:	other: EPIWIN (v3.11) MPBPWIN Submodel (v1.41); experimental database.	
<b>Year</b>	:	2003	
<b>GLP</b>	:		
<b>Test substance</b>	:	as prescribed by 1.1 - 1.4	
<b>Reliability</b>	:	(2) valid with restrictions	
15.12.2003			(16)
<b>Value</b>	:	= 11.5 °C	
<b>Sublimation</b>	:		
<b>Method</b>	:	other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); mean of Adapted Joback and Gold & Ogle methods	
<b>Year</b>	:	2003	
<b>GLP</b>	:		
<b>Test substance</b>	:	as prescribed by 1.1 - 1.4	
<b>Reliability</b>	:	(2) valid with restrictions	
15.12.2003			(16)
<b>Value</b>	:	= -10.4 °C	
<b>Sublimation</b>	:		
<b>Method</b>	:	other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); mean of Adapted Joback and Gold & Ogle methods	
<b>Year</b>	:	2003	
<b>GLP</b>	:		
<b>Test substance</b>	:	other TS	
<b>Test substance</b>	:	Isooctyl acrylate (CAS No. 29590-42-9)	
<b>Reliability</b>	:	(2) valid with restrictions	
15.12.2003			(16)

### 2.2 BOILING POINT

<b>Value</b>	:	= 158 °C at 66.7 hPa
<b>Decomposition</b>	:	

## 2. Physico-Chemical Data

Id 1330-61-6

Date 17.12.2003

<b>Method</b>	:		
<b>Year</b>	:		
<b>GLP</b>	:	no data	
<b>Test substance</b>	:	as prescribed by 1.1 - 1.4	
<b>Source</b>	:	Handbook data Rohm and Haas Company Spring House	
<b>Reliability</b>	:	(2) valid with restrictions	
<b>Flag</b>	:	Critical study for SIDS endpoint	
15.12.2003			(7)
<b>Value</b>	:	= 158 °C at	
<b>Decomposition</b>	:		
<b>Method</b>	:		
<b>Year</b>	:		
<b>GLP</b>	:	no data	
<b>Test substance</b>	:	as prescribed by 1.1 - 1.4	
<b>Source</b>	:	Handbook data Rohm and Haas Company Spring House	
<b>Reliability</b>	:	(2) valid with restrictions	
15.12.2003			(4)
<b>Value</b>	:	= 158 °C at 66.5 hPa	
<b>Decomposition</b>	:		
<b>Method</b>	:	other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); experimental database	
<b>Year</b>	:	2003	
<b>GLP</b>	:		
<b>Test substance</b>	:	as prescribed by 1.1 - 1.4	
<b>Reliability</b>	:	(2) valid with restrictions	
15.12.2003			(16)
<b>Value</b>	:	= 253.4 °C at	
<b>Decomposition</b>	:		
<b>Method</b>	:	other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); Adapted Stein and Brown Method	
<b>Year</b>	:	2003	
<b>GLP</b>	:		
<b>Test substance</b>	:	as prescribed by 1.1 - 1.4	
<b>Reliability</b>	:	(2) valid with restrictions	
15.12.2003			(16)
<b>Value</b>	:	= 196.8 °C at	
<b>Decomposition</b>	:		
<b>Method</b>	:	OECD Guide-line 103 "Boiling Point/boiling Range"	
<b>Year</b>	:		
<b>GLP</b>	:	yes	
<b>Test substance</b>	:	other TS	
<b>Remark</b>	:	IOA polymerises at elevated temperatures	
<b>Source</b>	:	3M Belgium B.V. Zwijndrecht EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	
<b>Test substance</b>	:	Isooctyl acrylate (CAS No. 29590-42-9)	
<b>Reliability</b>	:	(1) valid without restriction	

## 2. Physico-Chemical Data

Id 1330-61-6

Date 17.12.2003

15.12.2003 (18)

**Value** : = 216.9 °C at  
**Decomposition** :  
**Method** : other: EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); Adapted Stein and Brown Method  
**Year** : 2003  
**GLP** :  
**Test substance** : other TS

**Test substance** : Isooctyl acrylate (CAS No. 29590-42-9)  
**Reliability** : (2) valid with restrictions

16.12.2003 (16)

### 2.3 DENSITY

**Type** : density  
**Value** : = .885 at 20 °C  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** : as prescribed by 1.1 - 1.4

**Source** : Rohm and Haas Company Spring House  
**Reliability** : (4) not assignable

16.12.2003 (5)

#### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

**Value** : = .03 hPa at 25 °C  
**Decomposition** :  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** : as prescribed by 1.1 - 1.4

**Source** : Handbook data  
Rohm and Haas Company Spring House

**Reliability** : (2) valid with restrictions  
**Flag** : Critical study for SIDS endpoint

15.12.2003 (4)

**Value** : = .03 hPa at 25 °C  
**Decomposition** :  
**Method** : other (calculated): EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); mean VP of Antoine & Grain methods  
**Year** : 2003  
**GLP** :  
**Test substance** : as prescribed by 1.1 - 1.4

**Reliability** : (2) valid with restrictions

## 2. Physico-Chemical Data

Id 1330-61-6

Date 17.12.2003

17.12.2003

(16)

**Value** : = 1.333 hPa at 25 °C  
**Decomposition** :  
**Method** : OECD Guide-line 104 "Vapour Pressure Curve"  
**Year** :  
**GLP** : yes  
**Test substance** : other TS

**Source** : 3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

**Test substance** : Isooctyl acrylate (CAS No. 29590-42-9)

**Reliability** : (2) valid with restrictions

15.12.2003

**Value** : = .204 hPa at 25 °C  
**Decomposition** :  
**Method** : other (calculated): EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41); mean  
VP of Antoine & Grain methods

**Year** : 2003

**GLP** :

**Test substance** : other TS

**Test substance** : Isooctyl acrylate (CAS No. 29590-42-9)

**Reliability** : (2) valid with restrictions

17.12.2003

(16)

### 2.5 PARTITION COEFFICIENT

**Partition coefficient** :  
**Log pow** : = 5.07 at °C  
**pH value** :  
**Method** : other (calculated): EPIWIN (v 3.11); KOWWIN Submodel (v 1.67)  
**Year** : 2003  
**GLP** :  
**Test substance** : as prescribed by 1.1 - 1.4

**Reliability** : (2) valid with restrictions  
**Flag** : Critical study for SIDS endpoint

15.12.2003

(14)

**Partition coefficient** :  
**Log pow** : = 5.07 at °C  
**pH value** :  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** : as prescribed by 1.1 - 1.4

**Source** : Handbook data  
Rohm and Haas Company Spring House

**Reliability** : (2) valid with restrictions

15.12.2003

(4)

**Partition coefficient** :  
**Log pow** : = 3.93 at 25 °C

## 2. Physico-Chemical Data

Id 1330-61-6

Date 17.12.2003

pH value :  
Method : other (calculated)  
Year :  
GLP : no  
Test substance : other TS

Remark : The calculated log Pow for IOA agrees well with the measured value for 2-ethylhexyl acrylate, 3.67.

Source : 3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)  
Reliability : (2) valid with restrictions  
16.12.2003 (8)

Partition coefficient :  
Log pow : = 4.09 at °C  
pH value :  
Method : other (calculated): EPIWIN (v 3.11); KOWWIN Submodel (v 1.67)  
Year :  
GLP :  
Test substance : other TS

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)  
Reliability : (2) valid with restrictions  
15.12.2003 (14)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water  
Value : = 1.75 mg/l at 25 °C  
pH value :  
concentration : at °C  
Temperature effects :  
Examine different pol. :  
pKa : at 25 °C  
Description :  
Stable :  
Deg. product :  
Method : other: EPIWIN (v 3.11); WSKOWWIN Submodel (v 1.41)  
Year : 2003  
GLP :  
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions  
Flag : Critical study for SIDS endpoint  
17.12.2003 (17)

Solubility in :  
Value : = 1.75 mg/l at 25 °C  
pH value :  
concentration : at °C  
Temperature effects :  
Examine different pol. :  
pKa : at 25 °C  
Description :  
Stable :

## 2. Physico-Chemical Data

Id 1330-61-6

Date 17.12.2003

Deg. product	:		
Method	:		
Year	:		
GLP	:	no data	
Test substance	:	as prescribed by 1.1 - 1.4	
Source	:	Handbook data Rohm and Haas Company Spring House	
Reliability	:	(2) valid with restrictions	(4)
15.12.2003			
Solubility in	:	Water	
Value	:	= 12.44 mg/l at 23.1 °C	
pH value	:		
concentration	:	at °C	
Temperature effects	:		
Examine different pol.	:		
pKa	:	at 25 °C	
Description	:		
Stable	:		
Deg. product	:		
Method	:	OECD Guide-line 105	
Year	:		
GLP	:	yes	
Test substance	:	other TS	
Source	:	3M Belgium B.V. Zwijndrecht EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	
Test substance	:	Isooctyl acrylate (CAS No. 29590-42-9)	
Reliability	:	(1) valid without restriction	(18)
15.12.2003			
Solubility in	:	Water	
Value	:	= 16.8 mg/l at 25 °C	
pH value	:		
concentration	:	at °C	
Temperature effects	:		
Examine different pol.	:		
pKa	:	at 25 °C	
Description	:		
Stable	:		
Deg. product	:		
Method	:	other: EPIWIN (v 3.11); WSKOWWIN Submodel (v 1.41)	
Year	:	2003	
GLP	:		
Test substance	:	other TS	
Test substance	:	Isooctyl acrylate (CAS No. 29590-42-9)	
Reliability	:	(2) valid with restrictions	(17)
17.12.2003			

### 2.6.2 SURFACE TENSION

## 2. Physico-Chemical Data

**Id** 1330-61-6

**Date** 17.12.2003

### 2.7 FLASH POINT

**Value** : = 106 °C  
**Type** :  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** : as prescribed by 1.1 - 1.4  
  
**Source** : Rohm and Haas Company Spring House  
**Reliability** : (4) not assignable  
15.12.2003

(10)

### 2.8 AUTO FLAMMABILITY

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

### 2.11 OXIDIZING PROPERTIES

### 2.12 DISSOCIATION CONSTANT

### 2.13 VISCOSITY

### 2.14 ADDITIONAL REMARKS

## 3.1.1 PHOTODEGRADATION

Type : air  
 Light source :  
 Light spectrum : nm  
 Relative intensity : based on intensity of sunlight  
**DIRECT PHOTOLYSIS**  
 Half-life t<sub>1/2</sub> : = .5 day(s)  
 Degradation : % after  
 Quantum yield :  
 Deg. product :  
 Method : other (calculated): EPIWIN (v 3.11); AOPWIN Submodel (v 1.91)  
 Year : 2003  
 GLP :  
 Test substance : as prescribed by 1.1 - 1.4

Remark : Overall OH rate constant = 22.2E-12 cm<sup>3</sup>/molecule-sec  
 Half-life = 5.8 Hours (12-hr day; 1.5E6 OH/cm<sup>3</sup>)

Reliability : (2) valid with restrictions  
 Flag : Critical study for SIDS endpoint

17.12.2003 (11)

Type : air  
 Light source :  
 Light spectrum : nm  
 Relative intensity : based on intensity of sunlight  
**DIRECT PHOTOLYSIS**  
 Half-life t<sub>1/2</sub> : = .6 day(s)  
 Degradation : % after  
 Quantum yield :  
 Deg. product :  
 Method : other (calculated): EPIWIN (v 3.11); AOPWIN Submodel (v 1.91)  
 Year : 2003  
 GLP :  
 Test substance : other TS

Remark : Overall OH rate constant = 19.4E-12 cm<sup>3</sup>/molecule-sec  
 Half-life = 6.6 Hours (12-hr day; 1.5E6 OH/cm<sup>3</sup>)

Test substance : Isooctyl acrylate (CAS No. 29590-42-9)  
 Reliability : (2) valid with restrictions

17.12.2003 (11)

## 3.1.2 STABILITY IN WATER

Type : abiotic  
 t<sub>1/2</sub> pH4 : at °C  
 t<sub>1/2</sub> pH7 : = 10.6 year at 25 °C  
 t<sub>1/2</sub> pH9 : at °C  
 t<sub>1/2</sub> pH 8 : = 1.1 year at 25 °C  
 Deg. product :  
 Method : other (calculated): EPIWIN (v 3.11); HYDROWIN Submodel (v 1.67)  
 Year : 2003  
 GLP :

### 3. Environmental Fate and Pathways

Id 1330-61-6

Date 17.12.2003

**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : Rate constant: Total Kb for pH>8 at 25 deg C = 2.071E-002  
L/mol-sec

**Reliability** : (2) valid with restrictions  
17.12.2003

(13)

#### 3.1.3 STABILITY IN SOIL

#### 3.2.1 MONITORING DATA

#### 3.2.2 FIELD STUDIES

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

#### 3.3.2 DISTRIBUTION

**Media** : other: 1000 kg/hr emission to air  
**Method** : Calculation according Mackay, Level III  
**Year** : 2003

**Method** : The EPIWIN model was run using the following estimated  
physical/chemical properties: Henry's LC: 0.0012 atm-m<sup>3</sup>/mole; VP:  
0.0227 mmHg; and Log Kow: 5.07.

**Remark** : Level III Fugacity Model (Full-Output):

=====

Chem Name: 2-Propenoic acid, isodecyl ester

Molecular Wt: 212.34

Henry's LC: 0.0012 atm-m<sup>3</sup>/mole (Henrywin program)

Vapor Press: 0.0227 mm Hg (Mppbwin program)

Log Kow: 5.07 (Kowwin program)

Soil Koc: 4.82e+004 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	96.3	10.8	1000
Water	1.58	360	0
Soil	1.05	360	0
Sediment	1.03	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.54e-011	865	134	86.5	13.4
Water	5.77e-012	0.424	0.22	0.0424	0.022
Soil	3.97e-014	0.281	0	0.0281	0
Sediment	1.74e-012	0.0687	0.00286	0.00687	0.000286

Persistence Time: 13.9 hr

Reaction Time: 16.1 hr

### 3. Environmental Fate and Pathways

Id 1330-61-6

Date 17.12.2003

Advection Time: 104 hr  
Percent Reacted: 86.6  
Percent Advected: 13.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 10.75

Water: 360

Soil: 360

Sediment: 1440

Biowin estimate: 2.870 (weeks )

Advection Times (hr):

Air: 100

Water: 1000

Sediment: 5e+004

**Result**

: Concentration (%):

Air = 96

Water = 1.6

Soil = 1.1

Sediment = 1.0

**Test substance**

: as prescribed by 1.1 - 1.4

**Reliability**

: (2) valid with restrictions

**Flag**

: Critical study for SIDS endpoint

17.12.2003

(15)

**Media**

: other: 1000 kg/hr emission to water

**Method**

: Calculation according Mackay, Level III

**Year**

: 2003

**Method**

: The EPIWIN model was run using the following estimated physical/chemical properties: Henry's LC: 0.0012 atm-m<sup>3</sup>/mole; VP: 0.0227 mmHg; and Log Kow: 5.07.

**Remark**

: Level III Fugacity Model (Full-Output):

=====

Chem Name: 2-Propenoic acid, isodecyl ester

Molecular Wt: 212.34

Henry's LC: 0.0012 atm-m<sup>3</sup>/mole (Henrywin program)

Vapor Press: 0.0227 mm Hg (Mppbpwin program)

Log Kow: 5.07 (Kowwin program)

Soil Koc: 4.82e+004 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.54	10.8	0
Water	59.7	360	1000
Soil	0.0168	360	0
Sediment	38.7	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	5.75e-012	322	49.9	32.2	4.99
Water	5.06e-009	372	193	37.2	19.3
Soil	1.48e-014	0.105	0	0.0105	0
Sediment	1.53e-009	60.4	2.51	6.04	0.251

Persistence Time: 324 hr

Reaction Time: 429 hr

### 3. Environmental Fate and Pathways

Id 1330-61-6

Date 17.12.2003

Advection Time: 1.32e+003 hr  
Percent Reacted: 75.4  
Percent Advected: 24.6

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 10.75

Water: 360

Soil: 360

Sediment: 1440

Biowin estimate: 2.870 (weeks )

Advection Times (hr):

Air: 100

Water: 1000

Sediment: 5e+004

**Result**

: Concentration (%):

Air = 1.5

Water = 60

Soil < 0.1

Sediment = 39

**Test substance**

: as prescribed by 1.1 - 1.4

**Reliability**

: (2) valid with restrictions

17.12.2003

(15)

**Media**

: other: 1000 kg/hr emission to air

**Method**

: Calculation according Mackay, Level III

**Year**

: 2003

**Method**

: The EPIWIN model was run using the following estimated physical/chemical properties: Henry's LC: 0.0006 atm-m<sup>3</sup>/mole; VP: 0.153 mmHg; and Log Kow: 4.09.

**Remark**

: Level III Fugacity Model (Full-Output):

=====

Chem Name: 2-Propenoic acid, isooctyl ester

Molecular Wt: 184.28

Henry's LC: 0.0006 atm-m<sup>3</sup>/mole (Henrywin program)

Vapor Press: 0.153 mm Hg (Mppbpwin program)

Log Kow: 4.09 (Kowwin program)

Soil Koc: 5.04e+003 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	95.7	12.2	1000
Water	2.94	360	0
Soil	1.09	360	0
Sediment	0.231	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.98e-011	849	149	84.9	14.9
Water	7.41e-012	0.883	0.459	0.0883	0.0459
Soil	2.53e-013	0.327	0	0.0327	0
Sediment	2.4e-012	0.0173	0.00072	0.00173	7.2e-005

Persistence Time: 15.6 hr

Reaction Time: 18.4 hr

Advection Time: 104 hr

### 3. Environmental Fate and Pathways

Id 1330-61-6

Date 17.12.2003

Percent Reacted: 85  
Percent Advected: 15

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 12.2

Water: 360

Soil: 360

Sediment: 1440

Biowin estimate: 2.932 (weeks )

Advection Times (hr):

Air: 100

Water: 1000

Sediment: 5e+004

**Result**

: Concentration (%):

Air = 96

Water = 2.9

Soil = 1.1

Sediment < 1.0

**Test substance**

: Isooctyl acrylate (CAS No. 29590-42-9)

**Reliability**

: (2) valid with restrictions

17.12.2003

(15)

**Media**

: other: 1000 kg/hr emission to water

**Method**

: Calculation according Mackay, Level III

**Year**

: 2003

**Method**

: The EPIWIN model was run using the following estimated physical/chemical properties: Henry's LC: 0.0006 atm-m<sup>3</sup>/mole; VP: 0.153 mmHg; and Log Kow: 4.09.

**Remark**

: Level III Fugacity Model (Full-Output):

=====

Chem Name: 2-Propenoic acid, isooctyl ester

Molecular Wt: 184.28

Henry's LC: 0.0006 atm-m<sup>3</sup>/mole (Henrywin program)

Vapor Press: 0.153 mm Hg (Mpbwin program)

Log Kow: 4.09 (Kowwin program)

Soil Koc: 5.04e+003 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.38	12.2	0
Water	90.5	360	1000
Soil	0.027	360	0
Sediment	7.1	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	7.38e-012	316	55.7	31.6	5.57
Water	3.42e-009	408	212	40.8	21.2
Soil	9.43e-014	0.122	0	0.0122	0
Sediment	1.11e-009	7.99	0.332	0.799	0.0332

Persistence Time: 234 hr

Reaction Time: 320 hr

Advection Time: 874 hr

Percent Reacted: 73.2

### 3. Environmental Fate and Pathways

Id 1330-61-6

Date 17.12.2003

Percent Advected: 26.8

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 12.2

Water: 360

Soil: 360

Sediment: 1440

Biowin estimate: 2.932 (weeks )

Advection Times (hr):

Air: 100

Water: 1000

Sediment: 5e+004

**Result** : Concentration (%):

Air = 2.4

Water = 91

Soil < 0.1

Sediment = 7.1

**Test substance** : Isooctyl acrylate (CAS No. 29590-42-9)

**Reliability** : (2) valid with restrictions

17.12.2003

(15)

#### 3.4 MODE OF DEGRADATION IN ACTUAL USE

#### 3.5 BIODEGRADATION

**Type** : aerobic

**Inoculum** : activated sludge, domestic

**Contact time** : 28 day(s)

**Degradation** : = 100 (±) % after 28 day(s)

**Result** : readily biodegradable

**Kinetic of testsubst.** : 5 day(s) = 72 %

15 day(s) = 100 %

%

%

%

**Deg. product** :

**Method** : OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"

**Year** :

**GLP** : no

**Test substance** : other TS: 2-Propenoic acid, isooctyl ester, Lot 1023, containing 10-15 ppm methylethylhydroquinone

**Remark** : The sodium benzoate reference solution showed dissolved oxygen losses of 56, 74 and >83% at 5, 15 and 28 days, respectively.

Average loss of IOA in the uninhibited samples was 72% after 5 days. Loss after 15 and 28 days was 100% at each of the concentrations (concentrations not mentioned). Dissolved oxygen levels declined in proportion to IOA levels.

In the inhibited samples, loss of IOA was 0.4, 30 and 6.9% at 5, 15 and 28 days, respectively, with no oxygen

### 3. Environmental Fate and Pathways

**Id** 1330-61-6

**Date** 17.12.2003

**Source** : depletion.  
3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)  
**Reliability** : (1) valid without restriction  
**Flag** : Critical study for SIDS endpoint  
15.12.2003 (18)

#### 3.6 BOD5, COD OR BOD5/COD RATIO

#### 3.7 BIOACCUMULATION

#### 3.8 ADDITIONAL REMARKS

## 4. Ecotoxicity

Id 1330-61-6

Date 17.12.2003

### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : other: laboratory test, no data on water renewal  
Species : Pimephales promelas (Fish, fresh water)  
Exposure period : 96 hour(s)  
Unit : mg/l  
NOEC : = .34  
LC50 : = .67  
Limit test :  
Analytical monitoring : yes  
Method : OECD Guide-line 203 "Fish, Acute Toxicity Test"  
Year :  
GLP : yes  
Test substance : other TS

Source : 3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test condition : Test species: Juvenile fathead minnows, mean length 1.6 cm.  
Test substance : Isooctyl acrylate (CAS No. 29590-42-9)  
Reliability : (1) valid without restriction  
Flag : Critical study for SIDS endpoint  
15.12.2003 (18)

Type :  
Species : other: fish  
Exposure period : 96 hour(s)  
Unit : mg/l  
LC50 : = .9 calculated  
Method : other: EPIWIN (v 3.11); ECOSAR Submodel (v 0.99g)  
Year :  
GLP :  
Test substance :

Test substance : as prescribed by 1.1 - 1.4  
Reliability : (2) valid with restrictions  
17.12.2003 (12)

### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :  
Species : Daphnia magna (Crustacea)  
Exposure period : 48 hour(s)  
Unit : mg/l  
NOEC : < .24  
EC50 : = .4  
Analytical monitoring : yes  
Method : OECD Guide-line 202  
Year :  
GLP : yes  
Test substance : other TS

Remark : Based on the initial measured concentrations, 48-h EC50 and NOEC values for Daphnia magna as determined from the acute

## 4. Ecotoxicity

Id 1330-61-6

Date 17.12.2003

immobilisation test were 0.77 mg/l and <0.56 mg/l, respectively.

Similarly, its 48-h EC50 and NOEC values, based on mean measured concentrations, were 0.40 mg/l and <0.24 mg/l, respectively.

**Source** : 3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)  
**Test condition** : Test species: Daphnia magna, less than 24-h old neonates.  
**Test substance** : Isooctyl acrylate (CAS No. 29590-42-9)  
Lot number 1419  
**Reliability** : (1) valid without restriction  
**Flag** : Critical study for SIDS endpoint

17.12.2003

(18)

**Type** :  
**Species** : other: Daphnid  
**Exposure period** : 48 hour(s)  
**Unit** : mg/l  
**EC50** : = .55 calculated  
**Method** : other: EPIWIN (v 3.11); ECOSAR Submodel (v 0.99g)  
**Year** :  
**GLP** :  
**Test substance** :

**Test substance** : as prescribed by 1.1 - 1.4

**Reliability** : (2) valid with restrictions

17.12.2003

(12)

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Species** :  
**Endpoint** : growth rate  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**NOEC** : = 1.7  
**EC50** : = 2.13  
**Limit test** :  
**Analytical monitoring** : no data  
**Method** : OECD Guide-line 201 "Algae, Growth Inhibition Test"  
**Year** :  
**GLP** : yes  
**Test substance** : other TS

**Source** : 3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)  
**Test substance** : Isooctyl acrylate (CAS No. 29590-42-9)  
**Reliability** : (1) valid without restriction  
**Flag** : Critical study for SIDS endpoint

15.12.2003

(18)

**Species** : other algae: Green algae  
**Endpoint** :  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**EC50** : = .066 calculated

## 4. Ecotoxicity

Id 1330-61-6

Date 17.12.2003

Method : other: EPIWIN (v 3.11); ECOSAR Submodel (v 0.99g)  
Year :  
GLP :  
Test substance :

Test substance : as prescribed by 1.1 - 1.4  
Reliability : (2) valid with restrictions  
17.12.2003

(12)

### 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

#### 4.5.1 CHRONIC TOXICITY TO FISH

#### 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia magna (Crustacea)  
Endpoint : reproduction rate  
Exposure period : 14 day(s)  
Unit : mg/l  
NOEC : = .51  
EC50 : = 1.99  
IC50 : = .97  
Analytical monitoring : yes  
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"  
Year :  
GLP : yes  
Test substance : other TS

Result : The results mentioned above were based on mean measured concentrations.

Based on initial measured concentrations:

NOEC = 0.79 mg/l

EC50 = 2.93 mg/l

IC50 = 1.50 mg/l

Source : 3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)  
Test condition : Test species: Daphnia magna (Crustacea), less than 24-h old neonates  
Test substance : 2-Propenoic acid, isooctyl ester (lot 3290)  
Reliability : (2) valid with restrictions  
Flag : Critical study for SIDS endpoint

17.12.2003

(18)

Species : Daphnia magna (Crustacea)  
Endpoint : reproduction rate  
Exposure period : 21 day(s)  
Unit : mg/l  
NOEC : < .13  
EC50 : = 1.61  
IC50 : = 1.02  
Analytical monitoring : yes  
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"

## 4. Ecotoxicity

Id 1330-61-6

Date 17.12.2003

**Year** :  
**GLP** : yes  
**Test substance** : other TS

**Result** : The results mentioned above were based on mean measured concentrations.  
  
Based on initial measured concentrations:  
  
NOEC < 0.20 mg/l  
EC50 = 2.62 mg/l  
IC50 = 1.72 mg/l

**Source** : 3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

**Test condition** : Test species: Daphnia magna (Crustacea), less than 24-h old neonates

**Test substance** : 2-Propenoic acid, isooctyl ester (CAS No. 29590-42-9)  
Lot 3290

**Reliability** : (2) valid with restrictions

**Flag** : Critical study for SIDS endpoint

17.12.2003 (18)

### 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

### 4.6.2 TOXICITY TO TERRESTRIAL PLANTS

### 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

### 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

### 4.7 BIOLOGICAL EFFECTS MONITORING

### 4.8 BIOTRANSFORMATION AND KINETICS

### 4.9 ADDITIONAL REMARKS

**5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION****5.1.1 ACUTE ORAL TOXICITY**

**Type** : LD50  
**Value** : > 5000 mg/kg bw  
**Species** : rat  
**Strain** : Sprague-Dawley  
**Sex** : male/female  
**Number of animals** : 10  
**Vehicle** :  
**Doses** : 5000 mg/kg bw  
**Method** : OECD Guide-line 401 "Acute Oral Toxicity"  
**Year** : 1989  
**GLP** : yes  
**Test substance** : other TS

**Method** : Test method: limit test  
 Five male and five female young adult albino rats, weighing between 228 and 288 g were fasted overnight and administered undiluted IOA monomer at a dose of 5000 mg/kg body weight by oral gavage. The animals were housed by sex in groups of five. The animals were observed for clinical signs and mortality for 1, 2.5 and 4 hours post-dosing, then daily for the 14 days following dosing, at which time they were sacrificed, weighed and subjected to gross necropsy.

**Result** : No treatment-related mortality occurred during the study. Average body weights for male and female rats increased by 43 and 13%, respectively, over the course of the study. Clinical signs consistent with gastrointestinal irritation (diarrhea) and mild central nervous system depression (ataxia and hypoactivity) were observed in most of the animals for the first two days after dosing. No significant gross lesions were noted at necropsy.

**Source** : 3M Belgium B.V. Zwijndrecht  
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

**Test condition** : Temperature and humidity of the animal room ranged from 18 to 23 degrees C and from 19 to 39%, respectively.

**Test substance** : Isooctyl acrylate (CAS No. 29590-42-9)

**Reliability** : (1) valid without restriction

**Flag** : Critical study for SIDS endpoint

17.12.2003

(1) (2)

**5.1.2 ACUTE INHALATION TOXICITY****5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES**

### 5.2.1 SKIN IRRITATION

### 5.2.2 EYE IRRITATION

### 5.3 SENSITIZATION

### 5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	dermal
Exposure period	:	6-8 weeks
Frequency of treatm.	:	daily
Post exposure period	:	not applicable
Doses	:	Phase I: 0, 1.0, 7.5 and 15%; Phase II: 0 and 25% (lowered to 20% after one week)
Control group	:	yes, concurrent vehicle
NOAEL	:	= 15 %
LOAEL	:	= 20 - %
Method	:	other: OECD Guideline 422
Year	:	1993
GLP	:	yes
Test substance	:	other TS
Method	:	<p>The study was conducted in two phases. Phase I evaluated the 1.0, 7.5 and 15% concentrations with the first control group and the second phase examined the 25/20% group with the second control group. The second phase was conducted due to a lack of effects in Phase I. Animals received daily dermal applications of IOA in acetone at a constant dose volume of 100 ul/day. In Phase II, marked irritation at the treatment site in the high dose group after one week of dosing was observed and, the IOA concentration for this group was lowered to 20% and the treatment site was moved to an adjacent area for the remainder of the study. The control groups were dosed similarly with 100 ul of acetone. The dermal route of exposure was used because it is the most likely route of occupational exposure.</p>

Each animal was dosed with the test solution for at least six hours/day for two weeks before mating and throughout mating until sacrifice at post-natal day 4. The fur was clipped from the dorsal intrascapular area of the trunk before initiation of treatment and as needed thereafter. The second treatment site for the high dose group was on the posterior portion of the dorsal surface. The dose was spread uniformly over the treatment site and a collar was applied for approximately six hours to avoid ingestion. During the exposure period, animals were singly housed; i.e. mating pairs were separated and pups removed from nesting cages.

Dosing solutions were prepared in acetone. Homogeneity and stability of the Isooctyl Acrylate in the acetone solutions was confirmed prior to the start of the study. Dosing solution concentrations were confirmed

throughout the study.

The animals were observed twice daily for mortality, moribundity, and signs of poor health or abnormal behavior as well as for signs of abnormal pregnancy for females during gestation.

Dermal irritation was scored for each animal before each application of the test material or carrier (except on Day 0) and on the day of necropsy. Because of the change in dose level and dose site for Group 6, both sites were scored daily. Females that were observed in the process of delivering at the time of dermal scoring were not scored on that day.

Individual body weight data for males were recorded on the first day of treatment, weekly thereafter, and on the day of necropsy. Females were weighed on the first day of treatment, weekly during premating, on presumed gestation days (gd) 0, 7, 14 and 20, on lactation days 0 and 4, and on the day of necropsy. Females that did not show positive mating were weighed weekly and on the day of sacrifice.

Individual food consumption data were recorded weekly during the premating phase. Food consumption was measured for mated females for presumed gd 0-7, 7-14 and 14-20 and for females that delivered litters for lactation days 0-4.

Hematology and clinical chemistry measurements were made for all adult males before sacrifice. The animals were fasted overnight prior to blood collection. The following hematology parameters were evaluated: RBC, hemoglobin, hematocrit, platelet count, WBC, MCH, MCHC, MCV, differential blood cell count and blood cell morphology. The following clinical chemistry measurements were made: glucose, urea, nitrogen, creatinine, total protein, albumin, globulin, total bilirubin, cholesterol, AST, ALT, GGT, calcium, inorganic phosphorus, sodium, potassium and chloride.

After removal and sacrifice of the pups, the parental animals were weighed and sacrificed. Females that did not deliver were sacrificed on presumed gd 26. A complete necropsy was performed for all adults. Uteri and ovaries were examined for implantations and corpora lutea. Uteri that appeared non-gravid were stained for confirmation of pregnancy. The following organs were weighed: epididymides, kidneys, liver, testes and thymus. The following tissues were preserved and examined histologically: adrenals, brain, heart, epididymides, kidneys, liver, ovaries, skin (treated and untreated), spleen, testes and grossly observed lesions.

Statistical Analyses: Levene's test was done to test for variance homogeneity. Transformation was used to stabilize the variance when homogeneity was not met. Analysis of variance [ANOVA] was done on the homogeneous or transformed data. If the ANOVA was significant, Dunnett's t-test was used for pairwise comparisons between groups. When no transformation established variance homogeneity at  $p < 0.001$ , the data were also examined by nonparametric techniques using the Wilcoxon-Mann-Whitney two-sample rank test. One-way ANOVA was used to analyze continuous data such as body weights, body weight changes, food consumption, clinical chemistry and hematology values (except red blood cell morphology).

**Result**

: There were no test material-related clinical observations or adverse effects on body weights, body weight changes or food consumption. In Phase I (0,

1.0, 7.5 and 15%), a brownish-orange discoloration of the skin at the dosing site was observed for both sexes in all dose groups in a non-dose-related manner. Only minimal skin irritation in a few animals was observed inconsistently during the study through Day 54. Due to the lack of a clear treatment-related effect, Phase II (0 and 25/20%) was conducted. During the first week of dosing at 25% IOA, slight to moderate erythema, edema, desquamation and fissuring were observed in both sexes. In addition, two males were observed with subcutaneous hemorrhage. Because of this irritation, the dose concentration was reduced to 20% for the remainder of the study and was applied to a different location on each animal. Overall, dermal irritation was noted in the high dose group and included slight to moderate erythema and slight desquamation for males and slight erythema, slight to moderate desquamation and slight fissuring for females. Minimally higher serum aspartate aminotransferase and alanine aminotransferase levels were noted in males in the high dose group. There were no significant differences from controls in terminal body weights, absolute organ weights, organ-to-body weight percentages or macroscopic or microscopic findings for any dose group.

Mean measured test concentrations during the 8-week study ranged from 97 to 112% of the nominal concentrations.

See also section 5.8

**Source** : 3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

**Test substance** : 2-Propenoic Acid, Isooctyl Ester, IOA (CAS No. 29590-42-9); Purity: 99.75%

**Reliability** : (1) valid without restriction

**Flag** : Critical study for SIDS endpoint

17.12.2003 (3)

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Ames test

**System of testing** : S. typhimurium TA1535, TA1537, TA1538, TA98 and TA100

**Test concentration** : Six concentrations ranging from 0.005 to 0.5 ul/plate

**Cytotoxic concentr.** : 5.0 ul/plate

**Metabolic activation** : with and without

**Result** : negative

**Method** : OECD Guide-line 471

**Year** : 1980

**GLP** : no

**Test substance** : other TS

**Method** : The assay was performed with and without Aroclor 1254-induced rat liver S9 homogenate (approx. 15 mg protein/plate) as a metabolic activation system. Tests were run in quadruplicate with six concentrations of IOA ranging from 0.005 to 0.5 ul/plate. These concentrations were selected on the basis of a preliminary toxicity range-finding study in which IOA was toxic to strain TA100 at a concentration of 5.0 ul/plate but not at concentrations ranging from 0.01 to 1.0 ul/plate. Dimethylsulfoxide (DMSO) was used as the solvent control for all test strains. Positive controls were 2-anthramine (all strains), sodium azide (TA1535 and TA100), 9-aminoacridine (TA1537) and 2-nitrofluorene (TA1538 and TA98).

## 5. Toxicity

**Id** 1330-61-6

**Date** 17.12.2003

<b>Remark</b>	: This test was performed at SRI International, Menlo Park, CA, USA, beginning in May 1980. Although the study was not conducted according to GLPs, any deviation from current practice is believed not to have materially influenced the overall findings of the study.
<b>Result</b>	: The highest IOA concentration tested, 0.5 ul/plate, produced pinpoint colonies, indicating toxicity, in strain TA100. The positive controls showed significant (greater than two-fold) increases in the number of revertant colonies per plate compared to the DMSO negative control. No significant increase in revertants was observed at any IOA concentration, either with or without metabolic activation. IOA was not mutagenic under the conditions of the study.
<b>Source</b>	: 3M Belgium B.V. Zwijndrecht EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
<b>Test substance</b>	: Isooctyl acrylate (CAS No. 29590-42-9); Purity: not stated.
<b>Reliability</b>	: (1) valid without restriction
<b>Flag</b>	: Critical study for SIDS endpoint
17.12.2003	(2) (9)
<b>Type</b>	: Mouse lymphoma assay
<b>System of testing</b>	: Mouse lymphoma cells, L5178Y TK+/-
<b>Test concentration</b>	: 10 concentrations ranging from 0.0015 to 0.11 ul/ml
<b>Cycotoxic concentr.</b>	:
<b>Metabolic activation</b>	: with and without
<b>Result</b>	: negative
<b>Method</b>	: OECD Guide-line 476
<b>Year</b>	: 1980
<b>GLP</b>	: yes
<b>Test substance</b>	: other TS
<b>Method</b>	: IOA monomer was evaluated for mutagenic activity in L5178Y TK+/- mouse lymphoma cells according to a modification of the method of Clive [Mutat. Res. 31, 17 (1975)]. The assay was performed with and without Aroclor 1254-induced rat liver S9 homogenate as the metabolic activation system. Triplicate tests were run with 10 concentrations of IOA ranging from 0.0015 to 0.02 ul/ml without activation and 0.0084 to 0.11 ul/ml with activation. These concentrations were selected on the basis of preliminary toxicity range finding studies. Dimethylsulfoxide (DMSO) was used as the solvent and negative control. Ethylmethanesulfonate (EMS) and 7,12-dimethylbenz(a)anthracene (DMBA) were positive controls for the nonactivated and activated cultures, respectively.
<b>Remark</b>	: This test was performed at EG&G Mason Research Institute, Rockville, MD, USA, beginning in May 1980.
<b>Result</b>	: Average cloning efficiencies of the DMSO negative controls were 75.8 and 76.2% for the nonactivated and activated cultures, respectively. Average suspension growth factors for the DMSO negative controls were 20.7 and 11.1 for the nonactivated and activated cultures, respectively. Suspension growth for the nonactivated IOA cultures ranged from 19 to 98% and for the activated IOA cultures from 23 to 124%. The lowest concentration producing cell toxicity was 0.063 ul/ml in cultures with metabolic activation and 0.0036 ul/ml in cultures without metabolic activation. The positive controls showed significant (greater than two-fold) increases in mutant frequency compared to the DMSO negative control. With metabolic activation, three IOA concentrations had mutant frequencies which were two-fold greater than the solvent control but these were considered to be within the range of experimental error. Dose-related increases in mutant frequencies were not observed in either the activated or nonactivated portions of the assay. IOA was not mutagenic under the conditions of the

## 5. Toxicity

Id 1330-61-6

Date 17.12.2003

**Source** : assay.  
: 3M Belgium B.V. Zwijndrecht  
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)  
**Test substance** : Isooctyl acrylate (CAS No. 29590-42-9); Purity: not stated.  
**Reliability** : (1) valid without restriction  
**Flag** : Critical study for SIDS endpoint  
17.12.2003 (2) (6)

### 5.6 GENETIC TOXICITY 'IN VIVO'

### 5.7 CARCINOGENICITY

#### 5.8.1 TOXICITY TO FERTILITY

#### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

#### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

**Type** : other  
**In vitro/in vivo** :  
**Species** : rat  
**Sex** : male/female  
**Strain** : Fischer 344  
**Route of admin.** : dermal  
**Exposure period** : 6-8 weeks  
**Frequency of treatm.** : Daily  
**Duration of test** : 56 Days  
**Doses** : Phase I: 0, 1.0, 7.5 and 15%; Phase II: 0 and 25% (lowered to 20% after one week)  
**Control group** : yes, concurrent vehicle  
**Method** : other: OECD Guideline 422  
**Year** : 1993  
**GLP** : yes  
**Test substance** : other TS

**Method** : The study was conducted in two phases. Phase I evaluated the 1.0, 7.5 and 15% concentrations with the first control group and the second phase examined the 25/20% group with the second control group. The second phase was conducted due to a lack of effects in Phase I. Animals received daily dermal applications of IOA in acetone at a constant dose volume of 100 ul/day. In Phase II, marked irritation at the treatment site in the high dose group after one week of dosing was observed and, the IOA concentration for this group was lowered to 20% and the treatment site was moved to an adjacent area for the remainder of the study. The control groups were dosed similarly with 100 ul of acetone. The dermal route of exposure was used because it is the most likely route of occupational exposure.

Each animal was dosed with the test solution for at least six hours/day for

two weeks before mating and throughout mating until sacrifice at post-natal day 4. The fur was clipped from the dorsal intrascapular area of the trunk before initiation of treatment and as needed thereafter. The second treatment site for the high dose group was on the posterior portion of the dorsal surface. The dose was spread uniformly over the treatment site and a collar was applied for approximately six hours to avoid ingestion. During the exposure period, animals were singly housed; i.e. mating pairs were separated and pups removed from nesting cages.

Dosing solutions were prepared in acetone. Homogeneity and stability of the Isooctyl Acrylate in the acetone solutions was confirmed prior to the start of the study. Dosing solution concentrations were confirmed throughout the study.

The animals were observed twice daily for mortality, moribundity, and signs of poor health or abnormal behavior as well as for signs of abnormal pregnancy for females during gestation.

Pairing was initiated after 14 days of dosing. Each female was paired with one male from the same group for a maximum of 14 days. Vaginal examinations were done daily during cohabitation, and the presence of sperm in the vaginal smear or a copulatory plug was considered evidence of positive mating. The day when such evidence was noted was designated gd 0. When mating was confirmed, the males and females were separated. Females that did not show evidence of mating were placed in nesting boxes after completion of the 2-week mating period.

Litter observations: On postnatal day (pnd) 0, the sex of each pup was determined and litter size was recorded. Each live pup was examined for external abnormalities and weighed. On pnd 4, the sex of each pup was determined and the litter size recorded. The pups were examined for external abnormalities and weighed individually before sacrifice. Following sacrifice, the pups were examined for cervical, thoracic or abdominal visceral abnormalities and then discarded. Abnormal tissues were preserved. Whenever possible, dead pups were examined for cervical, thoracic and abdominal visceral abnormalities and congenital abnormalities, then discarded.

After removal and sacrifice of the pups, the parental animals were weighed and sacrificed. Females that did not deliver were sacrificed on presumed gd 26. A complete necropsy was performed for all adults. Uteri and ovaries were examined for implantations and corpora lutea. Uteri that appeared non-gravid were stained for confirmation of pregnancy. The following organs were weighed: epididymides, kidneys, liver, testes and thymus. The following tissues were preserved and examined histologically: adrenals, brain, heart, epididymides, kidneys, liver, ovaries, skin (treated and untreated), spleen, testes and grossly observed lesions.

Statistical Analyses: Levene's test was done to test for variance homogeneity. Transformation was used to stabilize the variance when homogeneity was not met. Analysis of variance [ANOVA] was done on the homogeneous or transformed data. If the ANOVA was significant, Dunnett's t-test was used for pairwise comparisons between groups. When no transformation established variance homogeneity at  $p < 0.001$ , the data were also examined by nonparametric techniques using the Wilcoxon-Mann-Whitney two-sample rank test. One-way ANOVA was used to analyze continuous data such as body weights, body weight changes, food

	<p>consumption, clinical chemistry and hematology values (except red blood cell morphology), litter data and length of gestation. Reproduction indices (number inseminated, number pregnant, female fertility and gestation index) were analyzed by the Cochran-Armitage test for trend and departure and by a Fisher-Irwin exact test. One-way analysis of covariance was used to analyze the pup body width with the number of pups in the litter as the covariate. Groups were compared to their respective control group for Phases I and II.</p>
<b>Result</b>	<p>: There were no test material-related clinical observations or adverse effects on body weights, body weight changes or food consumption. In Phase I (0, 1.0, 7.5 and 15%), a brownish-orange discoloration of the skin at the dosing site was observed for both sexes in all dose groups in a non-dose-related manner. Only minimal skin irritation in a few animals was observed inconsistently during the study through Day 54. Due to the lack of a clear treatment-related effect, Phase II (0 and 25/20%) was conducted. During the first week of dosing at 25% IOA, slight to moderate erythema, edema, desquamation and fissuring were observed in both sexes. In addition, two males were observed with subcutaneous hemorrhage. Because of this irritation, the dose concentration was reduced to 20% for the remainder of the study and was applied to a different location on each animal. Overall, dermal irritation was noted in the high dose group and included slight to moderate erythema and slight desquamation for males and slight erythema, slight to moderate desquamation and slight fissuring for females.</p> <p>There were no treatment-related effects on male fertility, female fertility, mean days to mating, length of gestation, gestation length, pup viability, mean number of pups/litter or pup weights. There were no treatment-related findings at necropsy of the pups. Reproductive organ weight and histopathology findings for the adults were similar to controls. The reproductive and developmental NOAEL was 20%.</p>
<b>Source</b>	<p>: 3M Belgium B.V. Zwijndrecht EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)</p>
<b>Test substance</b>	<p>: 2-Propenoic Acid, Isooctyl Ester, IOA (CAS No. 29590-42-9); Purity: 99.75%</p>
<b>Reliability</b>	<p>: (1) valid without restriction</p>
<b>Flag</b>	<p>: Critical study for SIDS endpoint</p>
17.12.2003	(3)

## 5.9 SPECIFIC INVESTIGATIONS

## 5.10 EXPOSURE EXPERIENCE

## 5.11 ADDITIONAL REMARKS

### 6.1 ANALYTICAL METHODS

### 6.2 DETECTION AND IDENTIFICATION

## 7. Eff. Against Target Org. and Intended Uses

**Id** 1330-61-6  
**Date** 17.12.2003

**7.1 FUNCTION**

**7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED**

**7.3 ORGANISMS TO BE PROTECTED**

**7.4 USER**

**7.5 RESISTANCE**

**8.1 METHODS HANDLING AND STORING**

**8.2 FIRE GUIDANCE**

**8.3 EMERGENCY MEASURES**

**8.4 POSSIB. OF RENDERING SUBST. HARMLESS**

**8.5 WASTE MANAGEMENT**

**8.6 SIDE-EFFECTS DETECTION**

**8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER**

**8.8 REACTIVITY TOWARDS CONTAINER MATERIAL**

- (1) Glaza, S. M. (1989). Acute Oral Toxicity Study in Rats (OECD Guidelines). Unpublished report (study no. 81000694), dated February 14, 1989, for Minnesota Mining & Manufacturing Company, St. Paul, MN, USA; by Hazleton Laboratories, Inc., Madison, WI, USA.
- (2) Gordon, S.C., Zimmerman, D.D. and Griffith, F.D. (1991). Acute toxicity, genotoxicity and dermal carcinogenicity assessment of isooctyl acrylate. J. Toxicol. Environ. Health 34, 279-296.
- (3) Henwood, S. M. (1993). Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Study with 2-Propenoic Acid, Isooctyl Ester (IOA), in Rats via Dermal Application. Unpublished report (no. HWI6329-104), dated March 1, 1993, for 3M Company, St. Paul, MN, USA; by Hazleton Wisconsin, Inc., Madison, WI, USA.
- (4) Howard P.H. and Meylan W.M. (1997). Handbook of Physical Properties of Organic Chemicals. CRC Press Inc., Lewis Publishers, Boca Raton. p. 578.
- (5) HSDB - Hazardous Substances Data Bank. US Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington DC: US Government Printing Office, 1984-5.
- (6) Kirby, P. E. (1980). Evaluation of Test Article T-2476 (MRI#446) for Mutagenic Potential Employing the L5178Y TK+/- Mutagenesis Assay. Unpublished report dated July 17, 1980, for 3M Company, St. Paul, MN, USA; by EG&G Mason Research Institute, Rockville, MD, USA.
- (7) Lide, D.R. (1996). CRC Handbook of Chemistry and Physics. CRC Press, Boca Raton; p. 291.
- (8) Method of Hunter, R., Faulkner, L., Culver, F. and Hill, J. (1985). QSAR, structure-activity based chemical modeling and information software. Montana State University, Bozeman, MT, USA. Unpublished 3M data.
- (9) Mortelmans, K. E. and A. Pomeroy. (1980). In vitro Microbiological Assays of 3M Company's Compound T-2476ChR. Unpublished report (SRI Project no. LSC-8958) dated June 1980, for 3M Company, St. Paul, MN, USA; by SRI International, Menlo Park, CA, USA.
- (10) Sigma-Aldrich MSDS (1998).
- (11) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- (12) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; ECOSAR Version 0.99g; PC-Computer software developed by ECOSAR Program, Risk Assessment Division (7403), Washington, D.C.
- (13) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; HYDROWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

## 9. References

**Id** 1330-61-6

**Date** 17.12.2003

- (14) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- (15) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- (16) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- (17) U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; WSKOWWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
- (18) Unpublished 3M data.

### 10.1 END POINT SUMMARY

### 10.2 HAZARD SUMMARY

### 10.3 RISK ASSESSMENT

201-15031B2

OECD Screening Information Data Sets (SIDS)

Screening Information Data Set  
SIDS for High Production Volume Chemicals

Organisation for Economic Co-operation and Development

OECD Initial Assessment

Processed by IRPTC

International Register of Potentially Toxic Chemicals

VOLUME 1  
part 2

A Contribution To IPCS  
International Programme of Chemical Safety

February 1995

	Substance
Chemical Name	: 2-Propenoic acid, isooctyl ester
Common Name	: Isooctyl acrylate
CAS Number	: 29590-42-9

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End Point : IDENTIFIERS, PHYSICAL AND CHEMICAL  
PROPERTIES

Chemical Name : 2-Propenoic acid, isooctyl ester

Common Name : Isooctyl acrylate

CAS Number : 29590-42-9

Synonyms

Acrylic acid, isooctyl ester IOA

Properties & Definitions

Molecular Formula : C<sub>11</sub>H<sub>20</sub>O<sub>2</sub>

Molecular Weight : 184.2

Boiling Point : 196.8C

State : liquid

Flash Point : 91.0C

Density : 0.88

Vapour Pressure : 0.1333kPa (1.0mmHg) at 25C\*

Octanol/Water Partition : log Pow = 3.93 at 25C

Coefficient

Water Solubility : 12.44mg/l at 23.1C

Colour : Colourless

Additives : Methylethylhydroquinone (MEHQ) may be  
used as stabilizer at concentrations up  
to 20ppm.

Impurities : 2-Propenoic acid, isononyl esters 3.16%  
(w/w), 2-propenoic acid, isoheptyl  
esters 1.62% (w/w), acrylate/acrylic  
acid adducts 0.45 (w/w), isooctyl  
alcohol 0.32% (w/w), 2-propenoic acid,

isodecyl esters 0.05% (w/w), 2-propenoic acid, isohexyl esters 0.02 (w/w).

General Comments : IOA polymerizes at elevated temperatures. \*VP = 0.33kPa (2.5mmHg) at 50C is also reported. The calculated log Pow for IOA agrees well with the measured value for 2-ethylhexyl acrylate 367. Viscosity: 2cps. Reactivity: violent, polymerization may result on exposure to heat.

#### Overall Evaluation

#### EXPOSURE

General discussion: IOA is manufactured in the U.S. by a single company (3M, St. Paul, MN) as an intermediate used for the synthesis of acrylic polymers. IOA monomer is not sold commercially. One product containing unreacted IOA as a component is sold by 3M as a concrete sealer for use by professional tradespeople. The IOA monomer in this product, about 1000kg/year, is polymerized at the job site. Trace amounts of unreacted IOA (typically less than 0.1% by weight) are present in certain industrial and consumer products (e.g. adhesive tapes) sold by 3M.

Environmental exposure: waste monomer is incinerated in a hazardous waste incinerator. There is no intentional discharge to water. Airborne emissions from 3M facilities are less than 1ppm (the limit of detection) for expected worst case operations. Industrial and consumer products containing trace amounts of unreacted IOA may be landfilled or incinerated after use. IOA is rapidly biodegraded aerobically and is expected to be rapidly oxidized in the atmosphere.

Consumer exposure: there are no known consumer uses for IOA monomer. Trace residual amounts of unreacted IOA (typically less than 0.1% by weight) are present in certain consumer products sold by 3M.

Occupational exposure: approximately 200 3M employees work in areas in which exposure to IOA, either as the liquid or vapor, may occur. Certain processes involving IOA are open systems in which IOA vapor may be generated. Ventilation systems are used to keep IOA vapor concentrations below the 3M Exposure Guideline of 5ppm (8-hour TWA). This guideline was established in 1981 and is based on the TLV established by the ACGIH for ethyl acrylate. Air monitoring studies of 3M processing and manufacturing areas have typically indicated

airborne IOA concentrations to be less than 1ppm. impermeable gloves are required to be worn by all employees who may come into contact with unreacted IOA monomer.

## TOXICITY

Human toxicity: on acute exposure, IOA is practically non-toxic orally to rats and is slightly irritating to the eyes and skin of rabbits.

IOA is expected to be a weak skin sensitizer by analogy to other low molecular weight acrylate esters. Repeated dermal exposure to IOA caused no systemic toxicity or reproductive/developmental effects at doses which caused moderate dermal irritation. IOA is not genotoxic in vitro and did not cause an increased incidence of cancers in a limited dermal carcinogenicity study in mice.

Ecotoxicity: IOA is moderately to highly toxic to fathead minnows, daphnia, algae and bacteria. Bioconcentration is unlikely due to its rapid biodegradation and, by analogy to other acrylate esters, its rapid hydrolysis in vivo.

## INITIAL ASSESSMENT

The potential for human exposure to IOA is very limited and its toxicity is low. Based on its use and hazard profile, the only anticipated human health risks posed by IOA are possible eye and skin irritation and allergic contact dermatitis among workers involved in its production or use. These effects are mitigated by the use of gloves by workers who may come into contact with the material.

IOA is manufactured in the U.S. by a single company as an intermediate for the synthesis of acrylic polymers. About 1000kg/year of IOA monomer is sold as a component of a concrete sealing product which is polymerized at the job site. Waste monomer is incinerated. There is no intentional discharge of IOA to water. Although IOA is significantly toxic to aquatic organisms and bacteria it is readily biodegraded. Airborne IOA concentrations in emissions from processing operations are typically less than 1ppm. Small quantities of unreacted IOA monomer are expected to reach landfills as a trace residual contaminant of certain industrial and consumer products. Atmospheric oxidation of IOA is expected to be rapid. There are no known or anticipated exposures to terrestrial organisms.

## CONCLUSIONS AND RECOMMENDATIONS

Based on its low occupational exposure potential, its low toxicity in vitro and mammalian studies, its limited release to the environment

and its predicted rapid environmental biodegradation, IOA is considered a low priority for additional human health or environmental effects testing at this time.

#### Production - Trade

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Geographic Area : USA

General Comments : No non-confidential data available. The 3M company, St Paul, MN is believed to be the only manufacturer of IOA.

#### References

!SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

#### Uses

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Geographic Area : USA

#### Use

Quantity	Year	Comments.
----------	------	-----------

>99%		An intermediate for the synthesis of acrylic polymers.
------	--	--

1000 kg		A single product containing unreacted IOA as an intentional component is sold by 3M company as a concrete sealer for use by professional tradespeople.
---------	--	--

IOA in this product is  
polymerized on the job site.

<0.1%                      Trace amounts of unreacted  
IOA monomer are present in a  
number of industrial and  
consumer products (e.g.  
adhesive tapes sold by 3M  
company).

#### References

Secondary References : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)

#### Study

End Point : Pathway into the Environment and  
Environmental Fate.

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

#### Test Method and Conditions

Test method description : Method of Hunter, R., Faulkner, L,  
Culver, F., and Hill, J., 1985, QSAR,  
structure-activity based chemical  
modelling and information software.  
(Montana State University, Montana,  
U.S.A.)

#### Quantity Transported

Medium to Medium    Quantity    Time    Year    to Year

to AIR    <1.0 mg/l

For expected worst case operations. (Reported as <1.0ppm, which is  
the detection limit).

to AQ      FRESH

No intentional discharge to water.

to SOIL      WASTE

Unspecified small amounts of unreacted IOA monomer are expected to reach landfills as a trace residual contaminant of certain industrial and consumer products.

to AIR                      9.77%

According to "Neely 100-day partitioning pattern" (QSAR)

to AQ                      50.83%

According to "Neely 100-day partitioning pattern" (QSAR)

to SOIL      GRND              20-38%

According to "Neely 100-day partitioning pattern" (QSAR)

to SED                      19.02%

According to "Neely 100-day partitioning pattern" (QSAR)

#### References

Secondary Reference      :    !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)

#### Study

End Point                      :    HUMAN INTAKE AND EXPOSURE

Chemical Name               :    Isooctylacrylate

CAS Number                 :    29590-42-9

#### Evaluations

Evaluation text              :    3M is believed to be the only

manufacturer of IOA. It is estimated that approximately 200 3M employees work in areas in which exposure to IOA, either as the liquid or vapor, could occur. Certain processes involving IOA are open systems in which IOA vapor may be generated. Ventilation systems are used to keep IOA vapor concentrations below the 3M Exposure Guideline of 5ppm (8h TWA). Air monitoring studies of 3M processing and manufacturing areas have typically indicated airborne IOA concentrations to be less than 1 ppm. Impermeable gloves are required to be worn by all employees who may come into contact with unreacted IOA monomer.

#### References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

#### Study

End Point : BIODEGRADATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Geographic Area : USA

#### Test Subject

Organism Medium Specification

AQ

Test Substance

Impurities : Methylethylhydroquinone 10-15ppm

#### Test Method and Conditions

Test method description : OECD Guideline 301d. Closed system.

(An)aerobic : AEROB

#### Exposure

Exposure Period : 5-28 d

#### Test Results

Quantity	Time	Comments on result
72%	AV	5 d In the uninhibited samples. Dissolved oxygen levels declined in proportion to test substance levels.
100%	AV	15-28 d In the uninhibited samples. Dissolved oxygen levels declined in proportion to test substance levels.
0.4%	AV	5 d In the inhibited samples with no oxygen depletion.
30%	AV	15 d In the inhibited samples with no oxygen depletion.
6.9%	AV	28 d In the inhibited samples with no oxygen depletion

The sodium benzoate reference solution showed dissolved oxygen loss of 56, 74 and 83% at 5, 15, 28 days, respectively.

General Comments : Biodegradation results indicate that IOA (the test substance) is treatable in sewage systems.

#### References

Primary Reference : #UR3MD\*

Unpublished 3M Data

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)

Study

End Point : BIODEGRADATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Evaluations

Evaluation text : Information on treatability of the  
substance: biodegradation results  
indicate IOA is treatable in sewage  
systems,

References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)

Study

End Point : PHOTODEGRADATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Test Method and Conditions

Test method description : Estimate by the method of William Meylan  
and Philip Howard, 1990. Atmospheric  
oxidation program, version 1.10,  
Syracuse Research Corporation, Syracuse,  
N.Y., U.S.A.

#### Test Results

Quantity	Time	Comments on result
50%	6,5 d	Half life due to reaction with ozone at an ozone concentration of $7 \times 10^{11}$ mol/cm <sup>3</sup> .

#### References

Primary Reference : #UR3MD\*

Unpublished 3M Data

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

#### Study

End Point : HYDROLYSIS

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

#### Test Method and Conditions

Test method description : Estimated by the method of William Meylan and Philip Howard, 1990. Atmospheric oxidation Program, version 1.10. Syracuse Research Corporation, Syracuse, N.Y. U.S.A.

#### Test Results

Quantity	Time	Comments on result
50%	11 h	T/2 due to reaction with hydroxyl radical at a hydroxyl radical concentration of $5 \times 10^5$ mol/cm <sup>3</sup> .

(Half-life reported as 0.46 day).

#### References

Primary Reference : UR3MD\*

Unpublished 3M Data

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)

#### Study

End Point : BIOCONCENTRATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

#### Evaluations

Evaluation text : Bioaccumulation is not anticipated since  
IOA is biodegradable and similar  
acrylate esters are readily metabolized  
in vivo.

#### References

Secondary Reference : !SIDSP\*

OECD/SIDS, Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)

#### Study

End Point : MAMMALIAN ACUTE TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Species/strain/system : Sprague-Dawley strain

Dose / Concentration : 5000 mg/kg BW

#### Test Method and Conditions

Test method descriptions : 5 male and female rats were fasted overnight and administered undiluted substance monomer at a dose of 5g/kg body weight by oral gavage. OECD 401; GLP: YES

#### Test Results

Organism	Medium	Spec.	Route	Lifestage	Sex	Effect	Effect	Comments
----------	--------	-------	-------	-----------	-----	--------	--------	----------

RAT		ORL		ADULT		LD50		Rat oral LD50 was greater than 5g/kg body weight under the condition of the study.
-----	--	-----	--	-------	--	------	--	--

General Comments : Test results: no treatment-related mortality occurred during the study. Average body weights for male and female rats increased 43% and 13%, respectively, over the course of the study. Clinical signs consistent with gastrointestinal irritation (diarrhea) and mild central nervous system depression (ataxia and hypoactivity) were observed in most of the animals for the first two days after dosing. No significant gross lesions were noted at necropsy.

#### References

Primary Reference : JTEHD6

Gordon, S.C. et al. Journal of Toxicology and Environmental Health, 34, 279-296, (1991)

Secondary Reference : !SIDSP\*

OECD/SIDS, Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)

Study

End Point : MAMMALIAN TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
----------	--------	---------------	-------	-----------	-----	----------------	-----------------

RAT		SKN	ADULT				
-----	--	-----	-------	--	--	--	--

Species/strain/system : F344 rats strain

Test Substance

Vehicle - Solvent : Acetone

Test Method and Conditions

Test method description : OECD Combined Repeated Dose and  
Reproductive/Developmental Screening  
Test.

Exposure

Exposure Type : SHORT

Dose / Concentration : 1-25%

Exposure comments : Dermal application of 0%, 1%, 7.5%, 15%  
or 25% of the substance solution in  
acetone at a constant dose volume of  
100ul/day. Due to marked irritation at

the treatment site in the high dose group the concentration was lowered to 20% after one week.

#### Test Results

Organ	Effect	Rev.	OnSet	Affected in Sex	Exposed - Controls
-------	--------	------	-------	--------------------	--------------------

SKIN	IRRIT			M	
------	-------	--	--	---	--

CIRC

STRUC

Dermal irritation was observed in the high dose group and included slight to moderate erythema and slight desquamation.

SKIN	IRRIT			F	
------	-------	--	--	---	--

CIRC

STRUC

Dermal irritation was observed in the high dose group and included slight erythema, slight to moderate desquamation and slight fissuring.

BLOOD	BIOCH			M	
-------	-------	--	--	---	--

Minimally higher serum aspartate and alanine aminotransferases levels were observed in the high dose group.

General Comments : There were no significant differences (as compared with controls) in body weights, absolute organ weights, organ to body weights percentages, or macroscopic and microscopic findings for any dose group.

#### References

Primary Reference : #UR3MD\*

Unpublished 3M Data, (1992)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, 12, (1993)

#### Study

End Point : CARCINOGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

#### Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
----------	--------	---------------	-------	-----------	-----	----------------	-----------------

MOUSE		SKN	74-79 d	M	40/GROUP		
-------	--	-----	---------	---	----------	--	--

Species/strain/system : C3H/HeJ mice strain

#### Test Substance

Vehicle - Solvent : Acetone

#### Test Method and Conditions

Test method description : EPA recommendations for dermal screening  
for carcinogenesis of  
acrylates/methacrylates. GLP: NO.

#### Exposure

Exposure Type : LONG

Frequency : 3 x/wk

Dose/Concentration : 5 % v/v

Exposure comments : Carcinogenicity potential was studied in  
a lifetime dermal bioassay. 25ul of the

substance monomer or acetone (negative solvent control) were applied to shaved backs of the animals three days/week. Daily observation for mortality and monthly examination for skin lesions were done. Necropsy was performed on all animals.

#### Test Results

Organ	Effect	Rev.	OnSet	Affected in Sex	Exposed - Controls
-------	--------	------	-------	--------------------	--------------------

SKIN	CIRC			M	
------	------	--	--	---	--

CHNG

Gross and microscopic dermal lesions observed in the IOA-treatment group were: edema (1/39 animals), surface crusting (10/39), epidermal vesiculation (1/39), hyperkeratosis (27/39).

SKIN	STRUC				
------	-------	--	--	--	--

NEO

Epidermal hyperplasia (16/39) and benign melanoma (1/39) were reported.

NEF

No significant difference in mean survival time between treatment and control groups.

General Comments : Microscopic examination of the melanoma showed that the cells were well differentiated with no indication of nuclear or cytoplasmic pleomorphism or atypia. Study performed at Bushy Run Research Center, Export, PA in April 1979.

#### References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, 16-17,  
(1993)

Study

End Point : MUTAGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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BACT

VTR

Species/strain/system : Salmonella typhimurium strains: TA98,  
TA100, TA1535, TA1537 and TA1538.

Test Substance

Vehicle - Solvent : Dimethylsulfoxide (DMSO)

Test Method and Conditions

Test method descriptions : Essentially similar to OECD 471; GLP: NO

Exposure

Exposure Type : SHORT

Dose / Concentration : 0.005-0.5 ul/ PLATE

Exposure comments : Ames salmonella microsome assay with and  
without metabolic activation was  
performed in quadruplicate with 6  
concentrations. Negative controls were

run with DMSO and positive controls with  
2-anthramine, sodium azide,  
9-aminoacridine or 2-nitrofluorene.

#### Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
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#### CELL

The highest concentration tested: 0.5ul/plate, produced pinpoint colonies, (indication of toxicity), in strain TA100.

#### NEF

No significant increase in revertants were observed at any IOA concentration, either with or without metabolic activation.

General Comments : IOA was not considered mutagenic under the conditions of the study.

#### References

Primary Reference : JTEHD6

Gordon, S.C. et al. Journal of  
Toxicology and Environmental Health, 34,  
297-308, (1991)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, 12, (1993)

#### Study

End Point : MUTAGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

#### Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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FUNGT		VTR					
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Species/strain/system : Saccharomyces cerevisiae D3 strain

#### Test Substance

Vehicle - Solvent : DMSO

#### Test Method and Conditions

Test method descriptions : Testing for mitotic recombinogenic activity following the method of Zimmerman and Schwater. GLP: NO

#### Exposure

Exposure Type : SHORT

Dose / Concentration : 0.00005.0.05 % v/v

Exposure comments : Test with and without metabolic activation was run at seven concentrations of IOA, DMSO was used for negative control and 1,2,3,4-diepoxybutane for the positive control.

#### Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
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CELL

Toxic effect was observed at concentration of 0.05% with metabolic activation and at 0.01% without metabolic activation.

NEF

IOA was not mutagenic under the test conditions.

General Comments : Study performed at SRI international,  
Menlo Park, CA, in May 1980.

#### References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, 13-14,  
(1993)

#### Study

End Point : MUTAGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

#### Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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MOUSE			VTR				
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Species/strain/system : Mouse embryo C3H/10T1/2 cell line

#### Test Substance

Vehicle - Solvent : Acetone

#### Test Method and Conditions

Test method description : Cell transformation potential according  
to Bertram; GLP: YES. Transformation was

classified according to the criteria of  
Reznikoff.

#### Exposure

Dose / Concentration : 0.0049-0.039 ul/ml

Exposure comments : Four concentrations, 12  
plates/concentration. Acetone was used  
for the negative control tests and 7,12-  
dimethylbenz(a)anthracene for the  
positive control. (Cancer Res. 33, 3231,  
1973)

#### Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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#### NEF

No type II or type III transformed foci were observed in any of the  
IOA cultures.

#### CELL

Lowest concentration producing cell toxicity was 0.0098ul/ml, without  
metabolic activation.

General Comments : IOA did not cause morphological  
transformation of C3H/10T1/2 cells in  
this test system.

#### References

Primary Reference : CNREA8

Bertram. Cancer Research, 37, 514,  
(1977)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, 14, (1993)

Study

End Point : MUTAGENICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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MOUSE		VTR					
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Species/strain/system : Mouse lymphoma, L5178Y TK +/- cells

Test Substance

Vehicle - Solvent : Dimethylsulfoxide

Test Method and Conditions

Test method descriptions : According to a modification of the method of Clive and OECD 476. GLP: YES

Exposure

Dose / Concentration : 0.0015-0.11 ul/ml

Exposure comments : Mutagenic activity assay was performed with and without metabolic activation at concentrations 0.0084-0.11 ul/ml and 0.0015-0.02 respectively, (In triplicates). DMSO was used in the negative control. Ethylmethanesulfonate and 7,12-dimethylbenz(a)anthracene were used in the positive control.

Test Results

			Affected in		
Organ	Effect	Rev.	OnSet	Sex	Exposed - Controls

PHENO CHNG

One concentration without metabolic activation and three concentrations with metabolic activation had mutant frequencies which were two-fold greater than the solvent control. Dose related increases were not observed.

#### CELL

Lowest concentration producing cell toxicity was 0.063ul/ml, without metabolic activation was 0.0036ul/ml. IOA was not considered mutagenic under the conditions of the assay.

#### References

Primary Reference : MUREAV

Clive, D. and Spencer, J. F. S. Mutation  
Research, 31, 17, (1975)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, 15, (1993)

#### Study

End Point : IRRITATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

#### Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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RBT

SKN

Species/strain/system : New Zealand rabbits strain

#### Test Method and Conditions

Test method description : U.S. Federal Hazardous Substances Act  
test guidelines. 0.5ml undiluted samples  
to both abraded and intact skin. GLP:  
NO.

#### Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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SKIN CIRC

Slight erythema (no edema) was noted at each test site in all of the  
test animals at both the 1 and 48 hour examination.

SKIN IRRIT

The mean primary dermal irritation score was 1.0 at both examination  
times.

General Comments : Conclusions: IOA was slightly irritating  
under the conditions of the study.

#### References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, 11, (1993)

#### Study

End Point : IRRITATION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

RBT OCU ADULT

Species/strain/system : New Zealand rabbits

Test Method and Conditions

Test method description : U.S. Federal Hazardous Substances Act  
test guidelines. GLP: NO.

Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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EYE IRRIT

At the 1 hour examination all animals showed slight discharge from the treated eye and 4/6 had slight conjunctival swelling. No evidence of irritation was noted at any other examination time up to 7 days.

General Comments : IOA monomer was slightly irritating  
under the conditions of the study.

References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, 11, (1993)

Study

End Point : REPRODUCTION

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

#### Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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RAT		SKN					
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Species/strain/system : F344 rats

#### Test Substance

Vehicle - Solvent : Acetone

#### Test Method and Conditions

Test method description : OECD Combined Repeated Dose and Reproductive/Developmental Screening test. GLP: YES.

#### Exposure

Exposure Type : SHORT

Dose / Concentration : 1-25%

Exposure comments : Dermal application of 0%, 1%, 7.5%, 15% or 25% of IOA solution in acetone at a volume dose of 100ul/day. Due to marked irritation at the treatment site in the high dose group, the concentration was lowered to 2% after one week.

#### Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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NEF

F

No overt maternal toxicity was noted at any dose level tested. The no-observable-effect-level NOEL for reproductive and developmental testing was 20%\* IOA.

General Comments : \*Severe dermal irritation at infusion site precluded dosing at higher concentrations. For other dermal effects see the results of repeated dose toxicity testing

#### References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 17, (1993)

#### Study

End Point : AQUATIC ACUTE TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Species/strain/system : Fathead minnows juvenile (Pimephales promelas) mean length=1.6cm

Exposure Period : 96 h

#### Test Method and Conditions

Test method description : OECD Guideline 203

#### Test Results

Organism Medium Spec. Route Lifestage Sex Effect Effect Comments

FISH AQ FRESH

LC50 Lethal concentration LC50 = 0.67mg/l for 96h. NOEC (no observed effect concentration) = 0.34mg/l.

General Comments : Results based on mean measured concentration.

#### References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

#### Study

End Point : AQUATIC TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

#### Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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BACT	AQ	MARIN					
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Species/strain/system : Bacteria bioluminiscent (Photobacterium phosphorium)

#### Test Substance

Description of the test : Test substance: lot 1419 substance

#### Test Method and Conditions

Test method description : Microtox(R) Toxicity Analyser, Model 2055 (Microbics Corp.) which measures the reduction in bioluminescence of naturally occurring marine bacterium in response to chemical toxicant.

## Exposure

Exposure Period : 5-15 mi

Dose / Concentration : 0.034-0.27 mg/l

Exposure comments : Two separate tests were run with four concentrations of test substance, ranging from 0.034-0.27mg/l.

## Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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### CHNG

Inhibitory concentration IC50 for reduction in bioluminescence = 0.163mg/l for 5 minutes and 0.168mg/l for 15 minutes.

## References

Primary Reference : #UR3MD\*

Unpublished 3M Data

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

## Study

End Point : AQUATIC TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

## Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

CRUS AQ FRESH

Species/strain/system : Water flea (*Daphnia magna*), less than 24h old neonates

Test Substance

Description of the test : Test substance: lot 1419 substance

Test Method and Conditions

Test method description : OECD Guideline 202. GLP specified. Immobilization test.

Exposure

Exposure Type : ACUTE

Exposure Period : 48 h

Dose/Concentration : <0.24-0.77 mg/l

Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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BEHAV

EC50

Effective Concentration for immobilization, EC50 = 0.77mg/l for 48h (test result based on initial measured concentrations).  
EC50 = 0.40mg/l for 48h (test result based on mean measured concentrations).

BEHAV

## NOEC

No Observed Effect Concentration NOEC =  $< 0.56 \text{ mg/l}$  (test result based on initial measured concentrations). NOEC =  $< 0.24 \text{ mg/l}$  for 48h. (Test result based on mean measured concentrations).

## References

Primary Reference : #UR3MD\*

Unpublished 3M Data

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)

## Study

End Point : AQUATIC TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

## Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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CRUS	AQ	FRESH					
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Species/strain/system : Water flea (*Daphnia magna*), less than  
24h old neonates

## Test Substance

Description of the test : Test substance: lot 3290  
substance

### Test Method and Conditions

Test method description : OECD Guideline 202. GLP specified.

### Exposure

Exposure Type : LONG

Exposure Period : 14-21 d

Dose / Concentration :  $<0.13$ -2.93 mg/l

### Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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#### EC50

Effective Concentration, EC50 = 2.93mg/l for 14 days, EC50 = 2.62mg/l for 21 days. (Test results based on initial measured concentrations).

Inhibitory concentration IC50 = 1.50mg/l for 14 days. IC50 = 1.72mg/l for 21 days. (Test results based on initial measured concentrations).

#### NOEC

No Observed Effect Concentration NOEC = 0.79mg/l for 14 days. NOEC =  $<0.20$ mg/l for 21 days, (Test result based on initial measured concentrations).

#### EC50

EC50 = 1.99mg/l for 14 days. EC50 = 1.61mg/l for 21 days. (Test result based on mean measured concentrations).

IC50 = 0.97mg/l for 14 days. IC50 = 1.02mg/l for 21 days. (Test result based on mean measured concentrations).

#### NOEC

NOEC = 0.51mg/l for 14 days. NOEC =  $<0.13$ mg/l for 21 days. (Test result based on mean measured concentrations).

### References

Primary Reference : #UR3MD\*

Unpublished 3M Data

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)

Study

End Point : AQUATIC TOXICITY

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

Study type : LAB

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
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FISH	AQ	FRESH					
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Species/strain/system : Fathead minnows juvenile (Pimephales  
promelas) mean length=1.6cm

Test Method and Conditions

Test method description : OECD Guideline 203

Exposure

Exposure Period : 96 h

Test Results

Organ	Effect	Rev.	Affected in OnSet	Sex	Exposed - Controls
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## NOEC

No Observed Effect Concentration, NOEC = 0.34mg/l for 96h

General Comments : Test result based on mean measured concentrations.

## References

Secondary Reference : !SIDSP\*

OECD/SIDS Screening Information Data Set  
(SIDS) of OECD High Production Volume  
Chemicals Programme, (1993)

## Substance

Chemical Name : Isooctylacrylate

CAS Number : 29590-42-9

## Description

Option for disposal: all waste IOA monomer generated by 3M is incinerated in a hazardous waste incinerator. There is no intentional discharge to water. It is anticipated that consumer and industrial products containing trace amounts of unreacted IOA monomer (typically less than 0.1% by weight) may be landfilled or incinerated after their use.

## References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data  
Set (SIDS) of OECD High Production  
Volume Chemicals Programme, (1993)